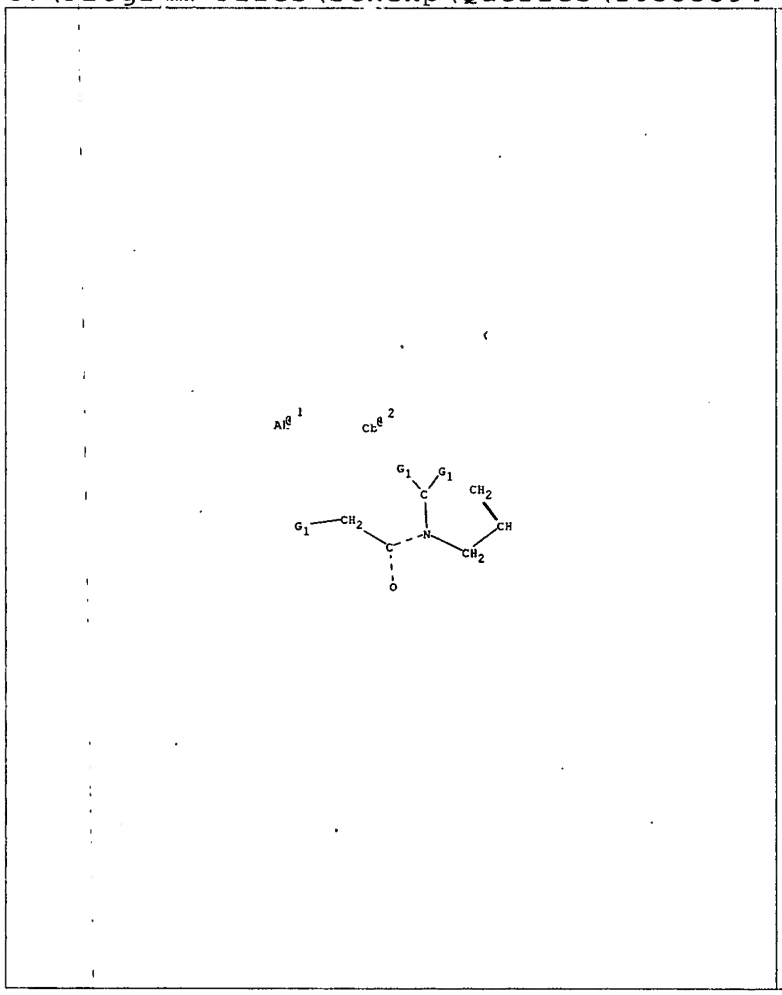
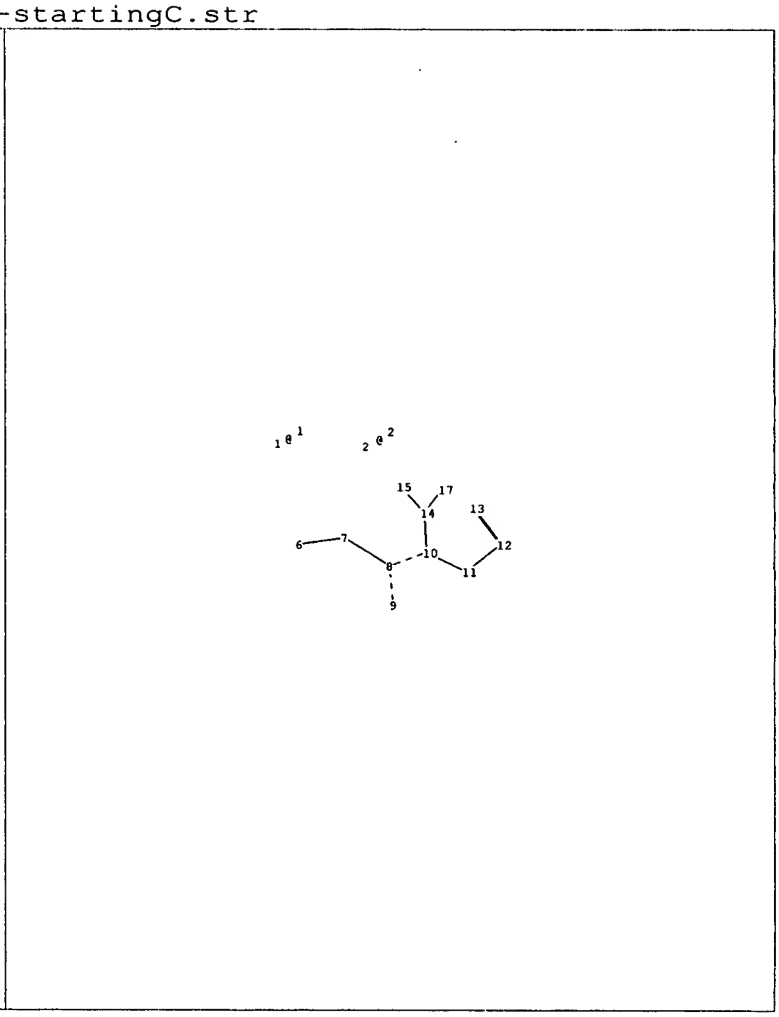
C:\Program Files\Stnexp\Queries\10553394-startingC.str





chain nodes :
1 2 6 7 8 9 10 11 12 13 14 15 17
chain bonds :
6-7 7-8 8-9 8-10 10-11 10-14 11-12 12-13 14-15 14-17
exact/norm bonds :
6-7 7-8 8-9 8-10 10-11 10-14 11-12 14-15 14-17
exact bonds :
12-13

G1:[*1],[*2]

Match level :
1:CLASS 2:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS
Generic attributes :
1:
Saturation : Saturated
2:
Saturation : Unsaturated

```
Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:ssptasjl1626

PASSWORD:
  * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'STNGUIDE' AT 09:50:13 ON 21 MAY 2007
FILE 'STNGUIDE' ENTERED AT 09:50:13 ON 21 MAY 2007
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.54     448.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00     -19.13

=> d his

     (FILE 'HOME' ENTERED AT 06:49:26 ON 21 MAY 2007)

     FILE 'REGISTRY' ENTERED AT 06:49:47 ON 21 MAY 2007
                ACT INC553394/A
               ---------
L1              STR
L2           804 SEA FILE=REGISTRY SSS FUL L1
               ---------
L3              STRUCTURE UPLOADED
L4              STRUCTURE UPLOADED
L5           727 S L4 SSS FULL SUB=L2
                SAV TEM IN6553394/A L5
L6             7 S L3 SSS FULL SUB=L2

     FILE 'CAPLUS' ENTERED AT 06:51:56 ON 21 MAY 2007
L7           236 S L5
L8             3 S L6

     FILE 'STNGUIDE' ENTERED AT 06:52:38 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 07:17:13 ON 21 MAY 2007
L9              STRUCTURE UPLOADED
L10            0 S L9
L11            4 S L9 SSS FULL

     FILE 'CASREACT' ENTERED AT 07:59:56 ON 21 MAY 2007
L12             STRUCTURE UPLOADED
L13            3 S L12

     FILE 'STNGUIDE' ENTERED AT 08:00:29 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:03:10 ON 21 MAY 2007
L14             STRUCTURE UPLOADED
L15            1 S L14
L16          106 S L12 SSS FULL
                SAV TEM 3PR553394/A L16 IMI553394/A
                ACT IMI553394/A
```

```
                ---------
L17               STR
L18           106 SEA FILE=CASREACT SSS FUL L17 (   799 REACTIONS)
                ---------
L19            37 S L14 SSS FULL SUB=L18

      FILE 'STNGUIDE' ENTERED AT 08:06:08 ON 21 MAY 2007

      FILE 'CASREACT' ENTERED AT 08:08:40 ON 21 MAY 2007
L20               STRUCTURE UPLOADED
L21               STRUCTURE UPLOADED
L22            19 S (L20 OR L21) SSS FULL SUB=L19

      FILE 'STNGUIDE' ENTERED AT 08:10:34 ON 21 MAY 2007

      FILE 'CASREACT' ENTERED AT 08:14:19 ON 21 MAY 2007

      FILE 'STNGUIDE' ENTERED AT 08:14:36 ON 21 MAY 2007

      FILE 'REGISTRY' ENTERED AT 09:41:11 ON 21 MAY 2007
L23               STRUCTURE UPLOADED

      FILE 'STNGUIDE' ENTERED AT 09:41:32 ON 21 MAY 2007

      FILE 'REGISTRY' ENTERED AT 09:41:55 ON 21 MAY 2007
L24             4 S L23

      FILE 'STNGUIDE' ENTERED AT 09:42:20 ON 21 MAY 2007

      FILE 'REGISTRY' ENTERED AT 09:43:51 ON 21 MAY 2007
L25               STRUCTURE UPLOADED
L26             1 S L25

      FILE 'STNGUIDE' ENTERED AT 09:44:14 ON 21 MAY 2007

=> d scan
'DISPLAY SCAN' IS NOT VALID IN CURRENT FILE

The DISPLAY SCAN command is not valid in the current file.
Enter HELP FORMATS and HELP DFIELDS to see valid DISPLAY
options in current file.

=> fil reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.54     448.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                 0.00     -19.13

FILE 'REGISTRY' ENTERED AT 09:50:26 ON 21 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   20 MAY 2007  HIGHEST RN 935426-16-7
DICTIONARY FILE UPDATES:  20 MAY 2007  HIGHEST RN 935426-16-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.
```

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

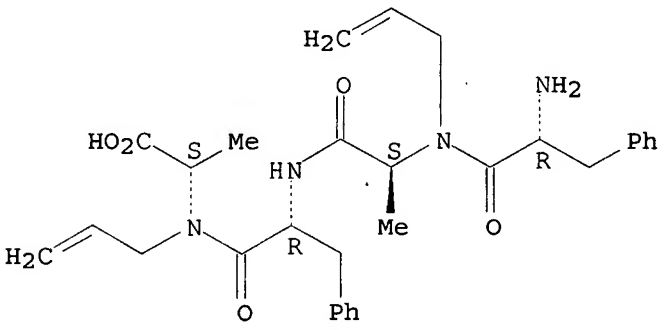
http://www.cas.org/support/stngen/stndoc/properties.html

=> d scan

L26 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN L-Alanine, D-phenylalanyl-N-2-propenyl-L-alanyl-D-phenylalanyl-N-2-propenyl- (9CI)
SQL 4
MF C30 H38 N4 O5

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l25 sss full
FULL SEARCH INITIATED 09:51:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 98339 TO ITERATE

100.0% PROCESSED 98339 ITERATIONS 201 ANSWERS
SEARCH TIME: 00.00.02

L27 201 SEA SSS FUL L25

=> sav tem str553394/a
ENTER L#, L# RANGE, ALL, OR (END):127

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	620.95
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-19.13

```
FILE 'STNGUIDE' ENTERED AT 09:51:48 ON 21 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.18     621.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00     -19.13

FILE 'REGISTRY' ENTERED AT 09:53:24 ON 21 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   20 MAY 2007  HIGHEST RN 935426-16-7
DICTIONARY FILE UPDATES:  20 MAY 2007  HIGHEST RN 935426-16-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-startingC.str

L28     STRUCTURE UPLOADED

=> d his

     (FILE 'HOME' ENTERED AT 06:49:26 ON 21 MAY 2007)

     FILE 'REGISTRY' ENTERED AT 06:49:47 ON 21 MAY 2007
                ACT INC553394/A
               ---------
L1              STR
L2           804 SEA FILE=REGISTRY SSS FUL L1
               ---------
L3              STRUCTURE UPLOADED
L4              STRUCTURE UPLOADED
L5           727 S L4 SSS FULL SUB=L2
                SAV TEM IN6553394/A L5
L6             7 S L3 SSS FULL SUB=L2
```

```
     FILE 'CAPLUS' ENTERED AT 06:51:56 ON 21 MAY 2007
L7          236 S L5
L8            3 S L6

     FILE 'STNGUIDE' ENTERED AT 06:52:38 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 07:17:13 ON 21 MAY 2007
L9                STRUCTURE UPLOADED
L10             0 S L9
L11             4 S L9 SSS FULL

     FILE 'CASREACT' ENTERED AT 07:59:56 ON 21 MAY 2007
L12               STRUCTURE UPLOADED
L13             3 S L12

     FILE 'STNGUIDE' ENTERED AT 08:00:29 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:03:10 ON 21 MAY 2007
L14               STRUCTURE UPLOADED
L15             1 S L14
L16           106 S L12 SSS FULL
                  SAV TEM 3PR553394/A L16 IMI553394/A
                  ACT IMI553394/A
                 ---------
L17               STR
L18           106 SEA FILE=CASREACT SSS FUL L17 (   799 REACTIONS)
                 ---------
L19            37 S L14 SSS FULL SUB=L18

     FILE 'STNGUIDE' ENTERED AT 08:06:08 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:08:40 ON 21 MAY 2007
L20               STRUCTURE UPLOADED
L21               STRUCTURE UPLOADED
L22            19 S (L20 OR L21) SSS FULL SUB=L19

     FILE 'STNGUIDE' ENTERED AT 08:10:34 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:14:19 ON 21 MAY 2007

     FILE 'STNGUIDE' ENTERED AT 08:14:36 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:41:11 ON 21 MAY 2007
L23               STRUCTURE UPLOADED

     FILE 'STNGUIDE' ENTERED AT 09:41:32 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:41:55 ON 21 MAY 2007
L24             4 S L23

     FILE 'STNGUIDE' ENTERED AT 09:42:20 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:43:51 ON 21 MAY 2007
L25               STRUCTURE UPLOADED
L26             1 S L25

     FILE 'STNGUIDE' ENTERED AT 09:44:14 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:50:26 ON 21 MAY 2007
L27           201 S L25 SSS FULL
                  SAV TEM STR553394/A L27

     FILE 'STNGUIDE' ENTERED AT 09:51:48 ON 21 MAY 2007
```

FILE 'REGISTRY' ENTERED AT 09:53:24 ON 21 MAY 2007
L28 STRUCTURE UPLOADED

=> s l28 sub=l27 sam
SAMPLE SUBSET SEARCH INITIATED 09:53:48 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 7 TO ITERATE

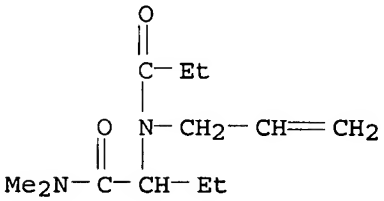
100.0% PROCESSED 7 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 7 TO 298
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 2 TO 124

L29 2 SEA SUB=L27 SSS SAM L28

=> d scan

L29 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Butyramide, 2-(N-allylpropionamido)-N,N-dimethyl- (5CI)
MF C12 H22 N2 O2

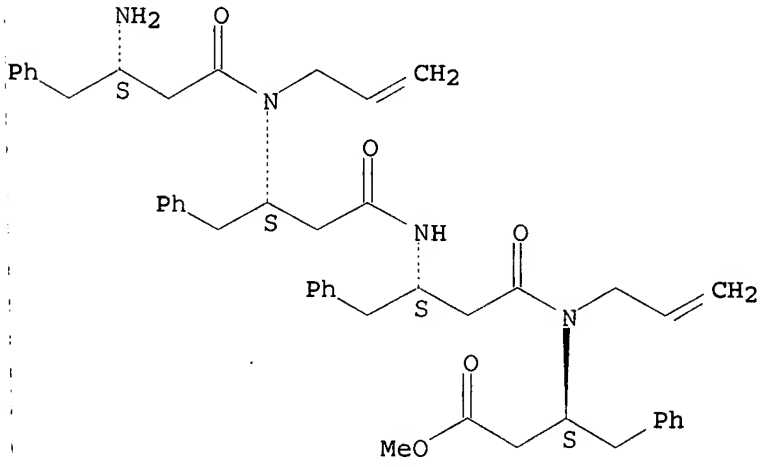


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L29 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzenebutanoic acid, β-[[(3S)-3-[[(3S)-3-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-1-oxo-4-phenylbutyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)- (9CI)
MF C47 H56 N4 O5

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	621.58

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-19.13

FILE 'STNGUIDE' ENTERED AT 09:54:12 ON 21 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	621.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-19.13

FILE 'REGISTRY' ENTERED AT 09:54:29 ON 21 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 20 MAY 2007 HIGHEST RN 935426-16-7
DICTIONARY FILE UPDATES: 20 MAY 2007 HIGHEST RN 935426-16-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d his

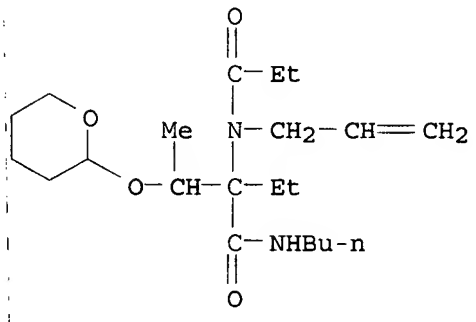
(FILE 'HOME' ENTERED AT 06:49:26 ON 21 MAY 2007)

FILE 'REGISTRY' ENTERED AT 06:49:47 ON 21 MAY 2007
ACT INC553394/A

```
                ---------
L1                STR
L2              804 SEA FILE=REGISTRY SSS FUL L1
                ---------
L3                STRUCTURE UPLOADED
L4                STRUCTURE UPLOADED
L5              727 S L4 SSS FULL SUB=L2
                  SAV TEM IN6553394/A L5
L6                7 S L3 SSS FULL SUB=L2

     FILE 'CAPLUS' ENTERED AT 06:51:56 ON 21 MAY 2007
L7              236 S L5
L8                3 S L6

     FILE 'STNGUIDE' ENTERED AT 06:52:38 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 07:17:13 ON 21 MAY 2007
L9                STRUCTURE UPLOADED
L10             0 S L9
L11             4 S L9 SSS FULL

     FILE 'CASREACT' ENTERED AT 07:59:56 ON 21 MAY 2007
L12               STRUCTURE UPLOADED
L13             3 S L12

     FILE 'STNGUIDE' ENTERED AT 08:00:29 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:03:10 ON 21 MAY 2007
L14               STRUCTURE UPLOADED
L15             1 S L14
L16           106 S L12 SSS FULL
                  SAV TEM 3PR553394/A L16 IMI553394/A
                  ACT IMI553394/A
                ---------
L17               STR
L18           106 SEA FILE=CASREACT SSS FUL L17 (   799 REACTIONS)
                ---------
L19            37 S L14 SSS FULL SUB=L18

     FILE 'STNGUIDE' ENTERED AT 08:06:08 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:08:40 ON 21 MAY 2007
L20               STRUCTURE UPLOADED
L21               STRUCTURE UPLOADED
L22            19 S (L20 OR L21) SSS FULL SUB=L19

     FILE 'STNGUIDE' ENTERED AT 08:10:34 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:14:19 ON 21 MAY 2007

     FILE 'STNGUIDE' ENTERED AT 08:14:36 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:41:11 ON 21 MAY 2007
L23               STRUCTURE UPLOADED

     FILE 'STNGUIDE' ENTERED AT 09:41:32 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:41:55 ON 21 MAY 2007
L24             4 S L23

     FILE 'STNGUIDE' ENTERED AT 09:42:20 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:43:51 ON 21 MAY 2007
L25               STRUCTURE UPLOADED
```

```
L26           1 S L25

     FILE 'STNGUIDE' ENTERED AT 09:44:14 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:50:26 ON 21 MAY 2007
L27         201 S L25 SSS FULL
                SAV TEM STR553394/A L27

     FILE 'STNGUIDE' ENTERED AT 09:51:48 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:53:24 ON 21 MAY 2007
L28             STRUCTURE UPLOADED
L29           2 S L28 SAM SUB=L27

     FILE 'STNGUIDE' ENTERED AT 09:54:12 ON 21 MAY 2007

     FILE 'REGISTRY' ENTERED AT 09:54:29 ON 21 MAY 2007

=> s l28 sub=l27 sss full
FULL SUBSET SEARCH INITIATED 09:54:46 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      201 TO ITERATE

100.0% PROCESSED      201 ITERATIONS                              49 ANSWERS
SEARCH TIME: 00.00.01

L30           49 SEA SUB=L27 SSS FUL L28

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               41.10     662.74

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00     -19.13

FILE 'CAPLUS' ENTERED AT 09:54:49 ON 21 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 21 May 2007  VOL 146 ISS 22
FILE LAST UPDATED: 20 May 2007  (20070520/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l30
L31           17 L30

=> d l31 tot bib abs hitstr
```

L31 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:661979 CAPLUS
DN 145:335862
TI A new highly convergent entry to densely functionalized aziridines based on the Ugi reaction
AU Banfi, Luca; Basso, Andrea; Guanti, Giuseppe; Paravidino, Monica; Riva, Renata
CS Dipartimento di Chimica e Chimica Industriale, Genoa, 16146, Italy
SO QSAR & Combinatorial Science (2006), 25(5-6), 457-460
CODEN: QCSSAU; ISSN: 1611-020X
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB The products of an Ugi-4CR employing lactate-derived O-protected α-hydroxycarbonyl derivs. underwent, during the subsequent O-deprotection reaction, an unexpected acyl migration from nitrogen to oxygen. After ester saponification, treatment of the resulting α-amino alc. with mesyl chloride gave rise to a regioselective and stereospecific cyclization to give a series of highly functionalized aziridines in good overall yield.
IT 909700-18-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(highly convergent entry to densely functionalized aziridines based on the Ugi reaction)
RN 909700-18-1 CAPLUS
CN Butanamide, N-butyl-2-ethyl-2-[(1-oxopropyl)-2-propenylamino]-3-[(tetrahydro-2H-pyran-2-yl)oxy]- (9CI) (CA INDEX NAME)



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:902331 CAPLUS
DN 141:379636
TI Process for preparation of optically active 2-allylcarboxylic acid derivatives
IN Okuro, Kazumi; Amano, Susumu; Kizaki, Noriyuki; Takesue, Teruaki; Mitsuda, Masaru; Ito, Noriyuki; Yasohara, Yoshihiko
PA Kaneka Corporation, Japan; Ono Pharmaceutical Co., Ltd.
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004092113	A1	20041028	WO 2004-JP5465	20040416

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1650187 A1 20060426 EP 2004-727979 20040416
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

US 2006223152 A1 20061005 US 2005-553394 20051214

PRAI JP 2003-114783 A 20030418

WO 2004-JP5465 W 20040416

OS MARPAT 141:379636

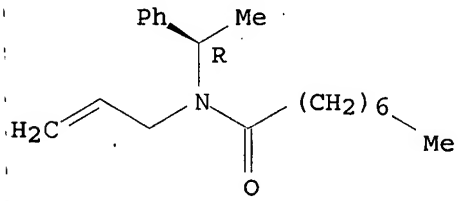
AB This invention pertains to a method for producing optically active 2-allylcarboxylic acid derivs., which comprises preparation of carboxamides, N-allylcarboxamides, rearrangement of allyl group, and hydrolysis processes. For example, (R)- and (S)-2-allyloctanoic acid were prepared starting from (R)-1-phenylethylamine and octanoyl chloride in good yield. This invention provides a method to prepare optically active 2-allylcarboxylic acid derivs. from less expensive starting materials with industrial advantages.

IT 781647-49-2P 781647-50-5P 781647-51-6P
781647-52-7P 781647-53-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of optically active 2-allylcarboxylic acid derivs.)

RN 781647-49-2 CAPLUS

CN Octanamide, N-[(1R)-1-phenylethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

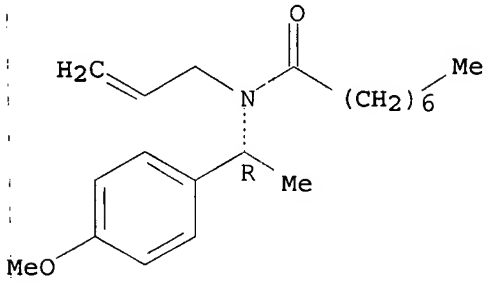
Absolute stereochemistry.



RN 781647-50-5 CAPLUS

CN Octanamide, N-[(1R)-1-(4-methoxyphenyl)ethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

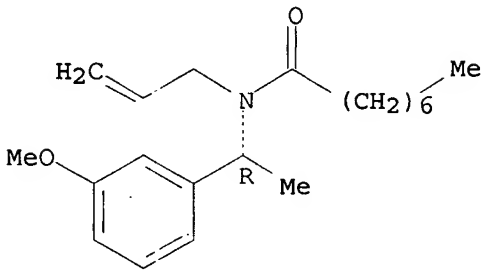
Absolute stereochemistry.



RN 781647-51-6 CAPLUS

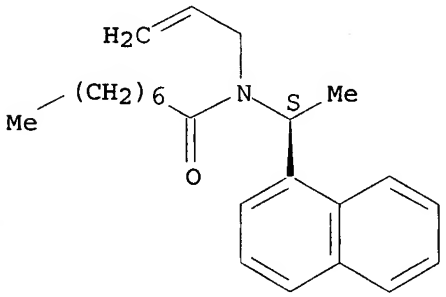
CN Octanamide, N-[(1R)-1-(3-methoxyphenyl)ethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



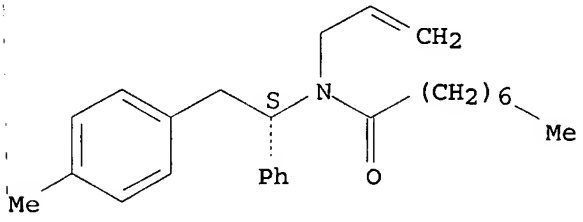
RN 781647-52-7 CAPLUS
CN Octanamide, N-[(1S)-1-(1-naphthalenyl)ethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 781647-53-8 CAPLUS
CN Octanamide, N-[(1S)-2-(4-methylphenyl)-1-phenylethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

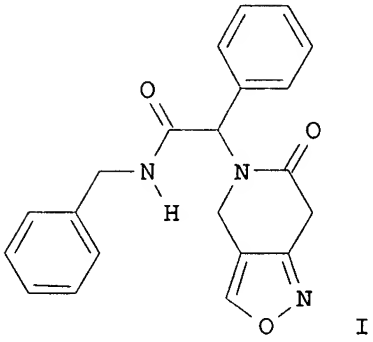
Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

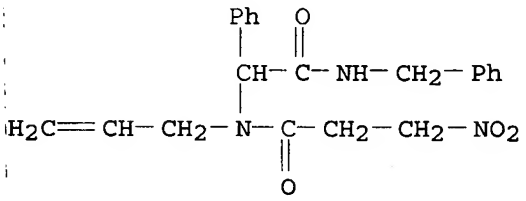
L31 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:277388 CAPLUS
DN 141:54228
TI Synthesis of novel fused isoxazoles and isoxazolines by sequential Ugi/INOC reactions
AU Akritopoulou-Zanze, Irini; Gracias, Vijaya; Moore, Joel D.; Djuric, Stevan W.
CS Scaffold-Oriented Synthesis, Abbott Laboratories, Abbott Park, IL, 60064-6099, USA

SO Tetrahedron Letters (2004), 45(17), 3421-3423
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 141:54228
GI



I

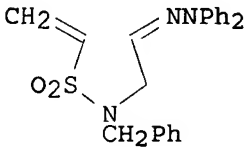
AB The synthesis of fused isoxazoles, e.g., I, and fused isoxazolines, by employing Ugi and intramol. nitrile oxide cycloaddn. synthetic sequence, is reported. The coupling of the multicomponent Ugi reaction with the intramol. N-oxide cyclization provided access to the heterocyclic ring systems in two steps, from easily available starting materials, in moderate to good overall yields.
IT 706814-39-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fused isoxazoles and isoxazoline via multicomponent Ugi reaction of aldehydes with primary amines, isocyanides, and nitroalkanoic acids followed by intramol. [3 + 2]-cycloaddn.)
RN 706814-39-3 CAPLUS
CN Benzeneacetamide, α-[(3-nitro-1-oxopropyl)-2-propenylamino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



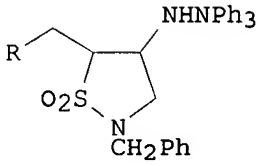
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:747158 CAPLUS
DN 139:307709
TI Indium-Mediated Tandem Radical Addition-Cyclization-Trap Reactions in Aqueous Media
AU Ueda, Masafumi; Miyabe, Hideto; Nishimura, Azusa; Miyata, Okiko; Takemoto, Yoshiji; Naito, Takeaki
CS Kobe Pharmaceutical University, Higashinada, Kobe, 658-8558, Japan
SO Organic Letters (2003), 5(21), 3835-3838
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society

DT Journal
LA English
OS CASREACT 139:307709
GI



I

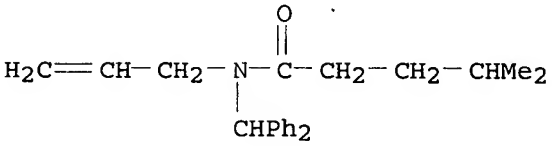


II

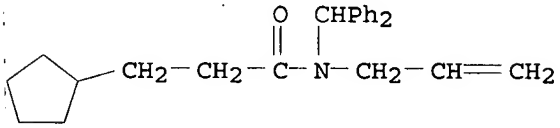
AB Tandem carbon-carbon bond-forming reactions were studied by using indium as a single-electron-transfer radical initiator. The radical addition-cyclization-trap reaction of a substrate having a vinyl sulfonamide group and an olefin moiety proceeded smoothly in aqueous media. The radical addition-cyclization reaction of a hydrazone (I) gave functionalized cyclic products (II; R = Me2CH, cyclopentyl, Me3C).

IT 610273-14-8P 610273-15-9P 610273-16-0P
RL: BYP (Byproduct); PREP (Preparation)
(isothiazolidine dioxides and pyrrolidinones via indium-mediated tandem radical addition-cyclization-trap reactions of unsatd. sulfonamides and carboxamides)

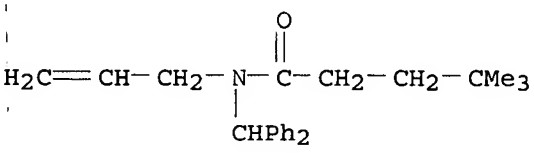
RN 610273-14-8 CAPLUS
CN Pentanamide, N-(diphenylmethyl)-4-methyl-N-2-propenyl- (9CI) (CA INDEX NAME)



RN 610273-15-9 CAPLUS
CN Cyclopentanepropanamide, N-(diphenylmethyl)-N-2-propenyl- (9CI) (CA INDEX NAME)

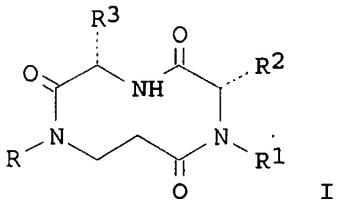


RN 610273-16-0 CAPLUS
CN Pentanamide, N-(diphenylmethyl)-4,4-dimethyl-N-2-propenyl- (9CI) (CA INDEX NAME)



RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

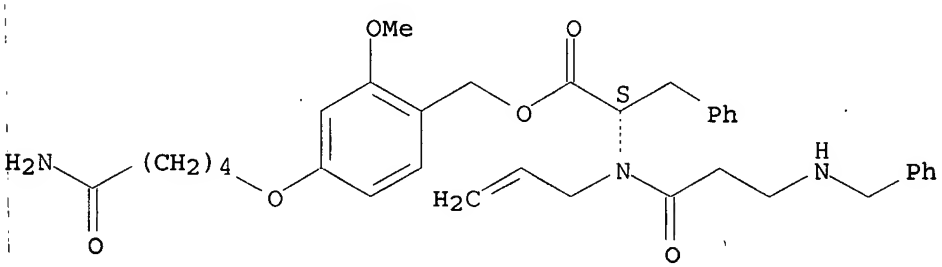
L31 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:417222 CAPLUS
DN 137:125386
TI Synthesis of Cyclic (α2β)-Tripeptides as Potential Peptide Turn Mimetics
AU Wels, Bas; Kruijtzer, John A. W.; Liskamp, Rob M. J.
CS Department of Medicinal Chemistry, Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Utrecht, 3508 TB, Neth.
SO Organic Letters (2002), 4(13), 2173-2176
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 137:125386
GI



I

AB The solid-supported synthesis followed by cyclization in solution of cyclic (α2β)-tripeptides, potential peptide β-turn mimetics, is described. The cyclization takes advantage of facilitating the rotation between trans- and cis-rotamers of two amide bonds. The method is amenable to combinatorial approaches as is illustrated by the synthesis of a small array of cyclic (α2β)-tripeptides [e.g., (I; R = PhCH2; R1 = CH2Ph, CH2-4-C6H4-OMe, CH2CH:CH2; R2 = CH2CH(CH3)2, CH2Ph; R3 = (CH3)3CO-4-C6H4-CH2, HO-4-C6H4-CH2, (CH3)3COCH2, (CH3)3COC(O)(CH2)2, Me, (CH3)3COC(O)NH(CH2)4)].
IT 444167-83-3DP, resin-bound 444167-84-4DP, resin-bound 444167-85-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of in the preparation of cyclic tripeptide β-turn mimetics using solid-phase techniques)
RN 444167-83-3 CAPLUS
CN L-Phenylalanine, N-(phenylmethyl)-β-alanyl-N-2-propenyl-, [4-[(5-amino-5-oxopentyl)oxy]-2-methoxyphenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

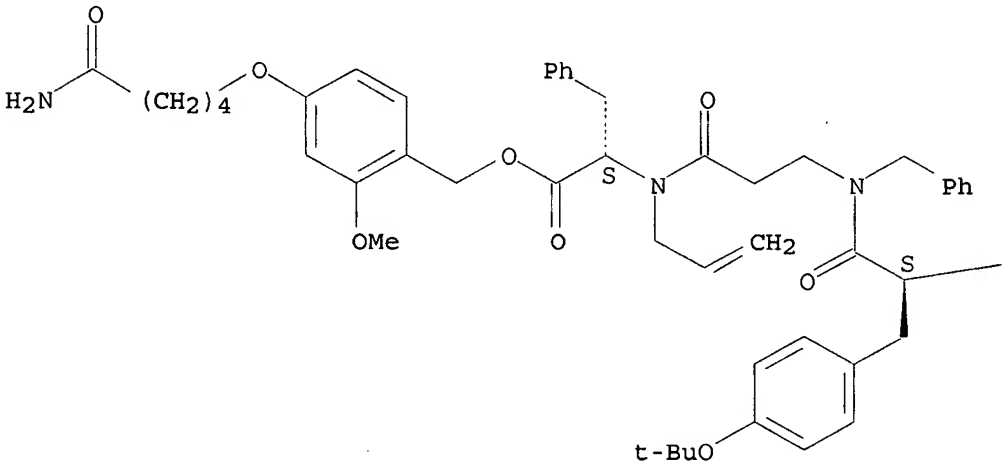


RN 444167-84-4 CAPLUS

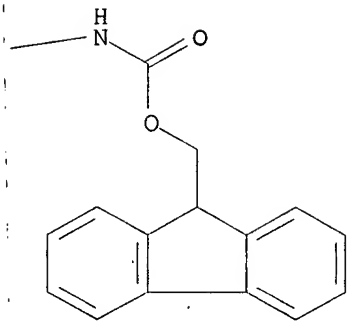
CN L-Phenylalanine, O-(1,1-dimethylethyl)-N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-tyrosyl-N-(phenylmethyl)-β-alanyl-N-2-propenyl-, [4-[(5-amino-5-oxopentyl)oxy]-2-methoxyphenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

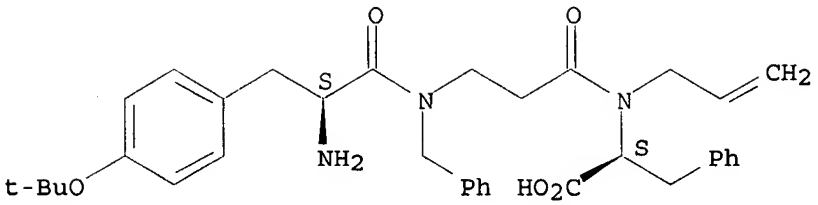


PAGE 1-B



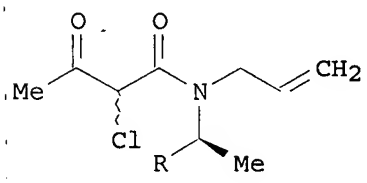
RN 444167-85-5 CAPLUS
CN L-Phenylalanine, O-(1,1-dimethylethyl)-L-tyrosyl-N-(phenylmethyl)-β-alanyl-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

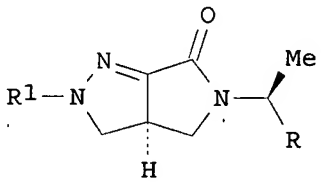


RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

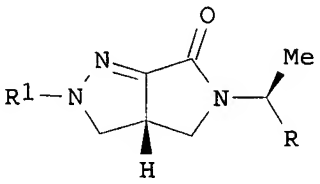
L31 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:925147 CAPLUS
DN 136:325475
TI Synthesis of enantiopure pyrrolo[3,4-c]pyrazole derivatives via intramolecular cycloaddition of homochiral nitrilimines
AU Broggini, Gianluigi; Molteni, Giorgio; Pilati, Tullio; Zecchi, Gaetano
CS Dipartimento di Scienze Chimiche, Fisiche e Matematiche, Universita dell'Insubria, Como, 22100, Italy
SO Synthetic Communications (2001), 31(24), 3799-3806
CODEN: SYNCAV; ISSN: 0039-7911
PB Marcel Dekker, Inc.
DT Journal
LA English
OS CASREACT 136:325475
GI



I



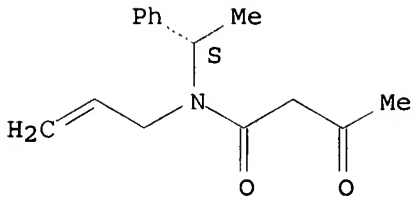
II



III

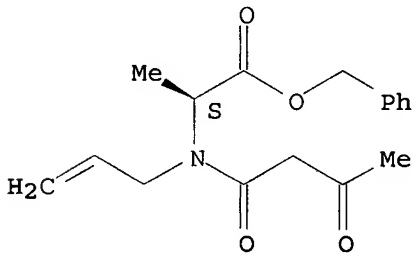
AB Intramol. cycloaddn. of homochiral nitrilimines, generated from the reaction of α-chloro acetoacetamides I (R = PhCO2CH2, Ph) with benzenediazonium chlorides, was exploited to obtain enantiopure pyrrolo[3,4-c]pyrazole derivs. II (R1 = 4-ClC6H4, 4-O2NC6H4) and III with high overall yields.
IT 186299-50-3P 413614-57-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolopyrazoles via intramol. cycloaddn. of homochiral nitrilimines)
RN 186299-50-3 CAPLUS
CN Butanamide, 3-oxo-N-[(1S)-1-phenylethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 413614-57-0 CAPLUS
CN L-Alanine, N-(1,3-dioxobutyl)-N-2-propenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

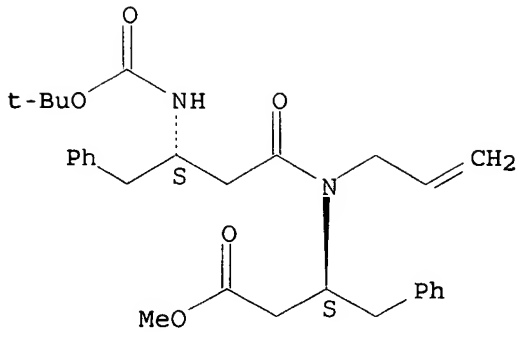
Absolute stereochemistry. Rotation (-).



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

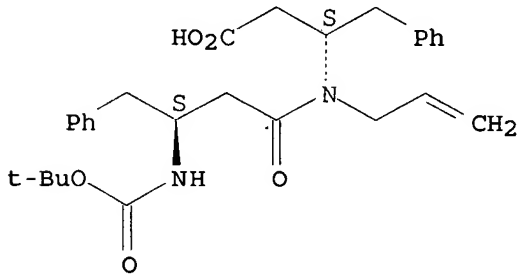
L31 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:677141 CAPLUS
DN 134:29682
TI Pseudoaxially Disubstituted Cyclo-β3-tetrapeptide Scaffolds
AU Sutton, P. W.; Bradley, A.; Farras, J.; Romea, P.; Urpi, F.; Vilarrasa, J.
CS Departament de Quimica Organica, Universitat de Barcelona, Barcelona, Catalonia, 08028, Spain
SO Tetrahedron (2000), 56(40), 7947-7958
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
AB An N,N-disubstituted cyclo-β3-tetrapeptide, identified as a potential mol. scaffold, has been synthesized on a multigram scale from β-homophenylalanine by employing a nosylate-based protection strategy. C2-Sym. derivs. containing pseudoaxial, combinatorially addressable functionalities have been prepared from the parent cyclopeptide.
IT 223595-66-2P 223595-67-3P 223595-69-5P
312311-60-7P 312311-61-8P 312311-62-9P
312311-63-0P 312311-65-2P 312311-70-9P
312311-71-0P 312311-72-1P 312311-73-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pseudoaxially disubstituted cyclo-β3-tetrapeptide scaffolds)
RN 223595-66-2 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



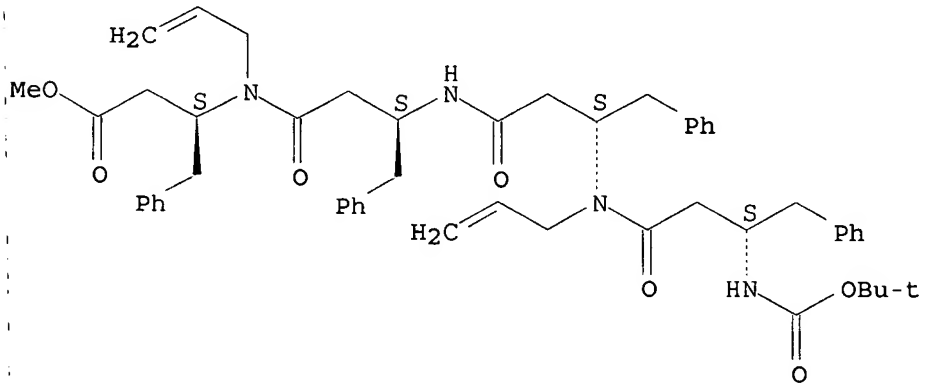
RN 223595-67-3 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



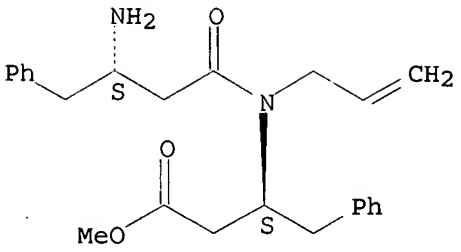
RN 223595-69-5 CAPLUS
CN 2,6,10,14-Tetraazaheptadecanedioic acid, 5,9,13-trioxo-3,7,11,15-tetrakis(phenylmethyl)-6,14-di-2-propenyl-, 1-(1,1-dimethylethyl) 17-methyl ester, (3S,7S,11S,15S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 312311-60-7 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

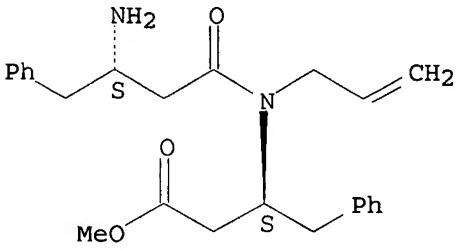


RN 312311-61-8 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

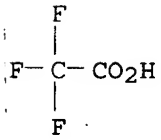
CRN 312311-60-7
CMF C24 H30 N2 O3

Absolute stereochemistry.



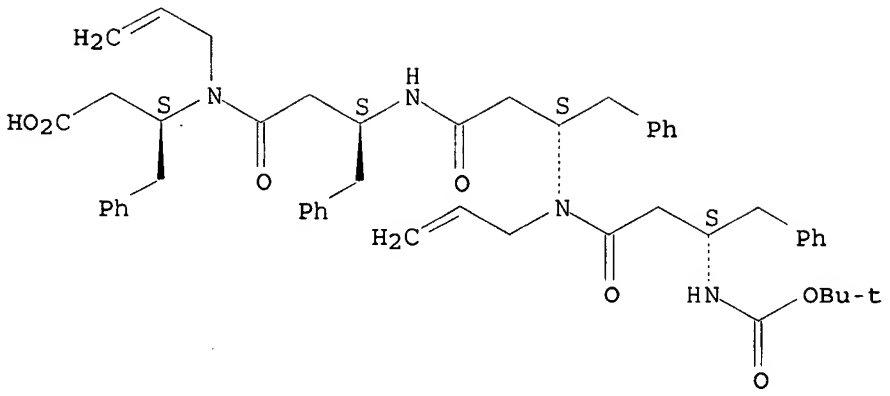
CM 2

CRN 76-05-1
CMF C2 H F3 O2



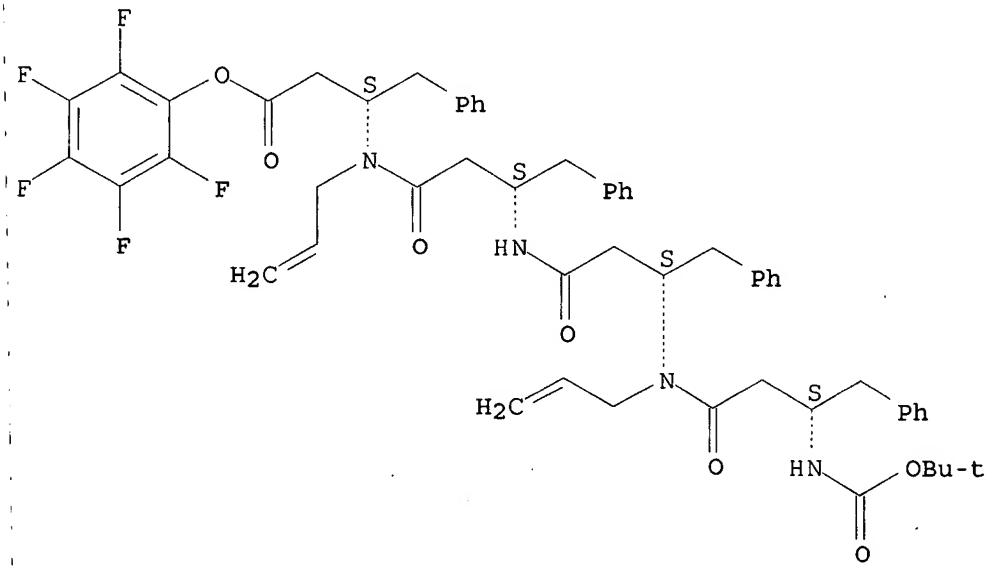
RN 312311-62-9 CAPLUS
CN 2,6,10,14-Tetraazaheptadecanedioic acid, 5,9,13-trioxo-3,7,11,15-tetrakis(phenylmethyl)-6,14-di-2-propenyl-, 1-(1,1-dimethylethyl) ester, (3S,7S,11S,15S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 312311-63-0 CAPLUS
CN 2,6,10,14-Tetraazaheptadecanedioic acid, 5,9,13-trioxo-3,7,11,15-tetrakis(phenylmethyl)-6,14-di-2-propenyl-, 1-(1,1-dimethylethyl) 17-(pentafluorophenyl) ester, (3S,7S,11S,15S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

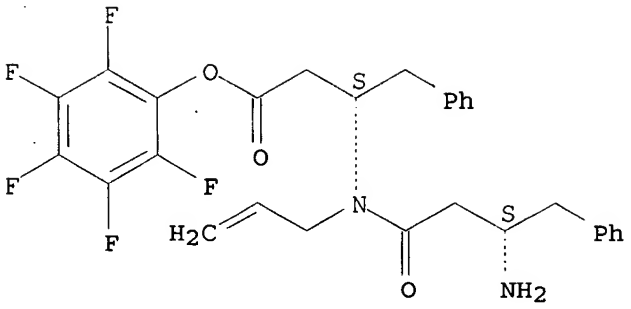


RN 312311-65-2 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-, pentafluorophenyl ester, (βS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

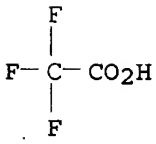
CRN 312311-64-1
CMF C29 H27 F5 N2 O3

Absolute stereochemistry.



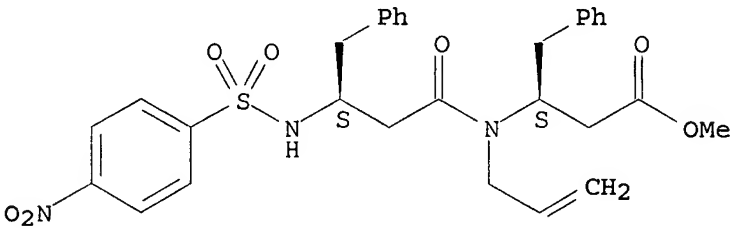
CM 2

CRN 76-05-1
CMF C2 H F3 O2



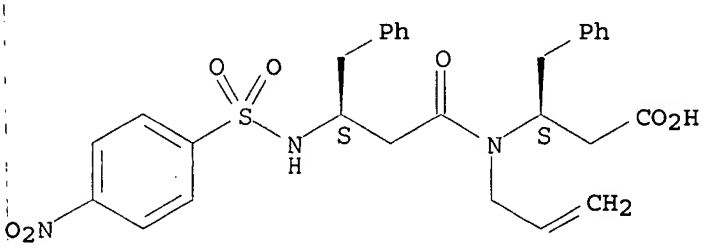
RN 312311-70-9 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(4-nitrophenyl)sulfonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 312311-71-0 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(4-nitrophenyl)sulfonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

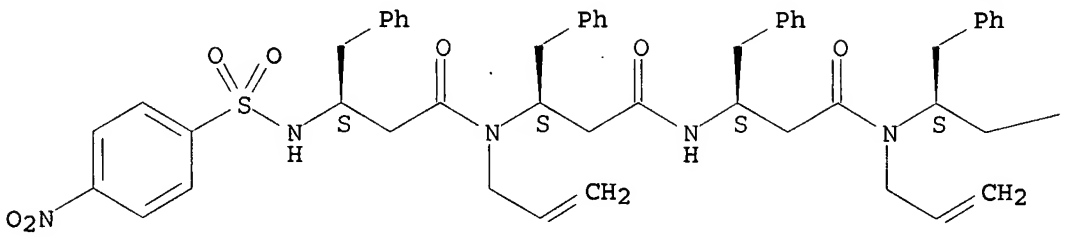


RN 312311-72-1 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(3S)-3-[[(3S)-3-[[(4-nitrophenyl)sulfonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-1-oxo-4-phenylbutyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester,

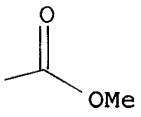
(βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

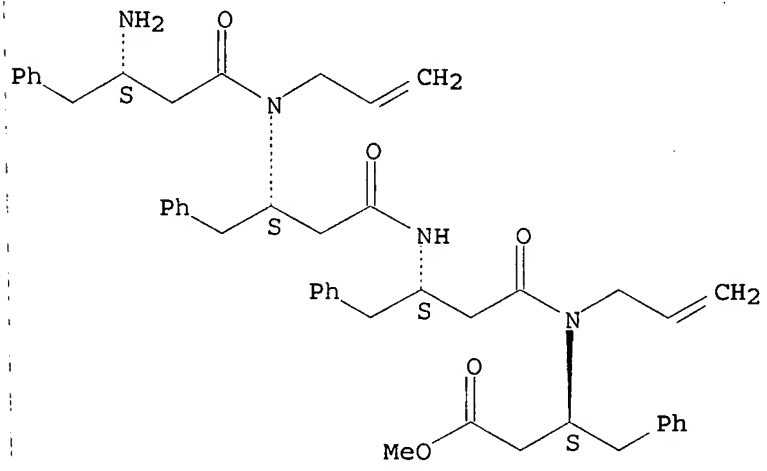


PAGE 1-B



RN 312311-73-2 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(3S)-3-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-1-oxo-4-phenylbutyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

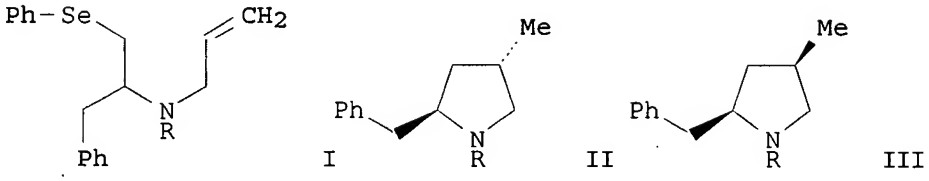
Absolute stereochemistry.



RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:281258 CAPLUS
DN 133:89393
TI Pyrrolidines from β-amino selenides via radical cyclization. Diastereoselectivity control by the N-substituent
AU Besev, Magnus; Engman, Lars
CS Department of Organic Chemistry Institute of Chemistry, Uppsala University, Uppsala, S-751 21, Swed.
SO Organic Letters (2000), 2(11), 1589-1592
CODEN: ORLEF7; ISSN: 1523-7060

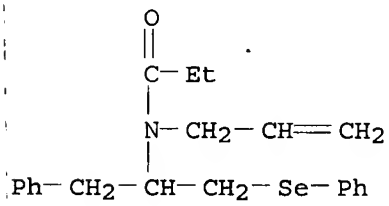
PB American Chemical Society
DT Journal
LA English
OS CASREACT 133:89393
GI



AB N-Allyl-β-aminoalkyl Ph selenides, precursors of 3-aza-5-hexenyl radicals, were prepared by ring opening of N-allylaziridines with benzeneselenol under acidic conditions or by NaBH3CN reduction of N-allylimines of α-phenylselenenyl ketones. The effect of various N-protective groups (acyl, sulfonyl, or phosphinoyl) on diastereoselectivity in thermally or photochem. initiated 3-aza-5-hexenyl reductive radical cyclization was studied. Whereas N-unprotected derivs. afforded trans-2,4-disubstituted pyrrolidines with good selectivity, the diphenylphosphinoyl group directed cyclization to occur in a highly cis-selective manner. Thus, radical cyclization of the (phenylselenylmethyl)phenylpropyl allylamine I (R = H) in benzene containing AIBN/Bu3SnH at 80° or in benzene at 15° with photolysis gave 92% of a 1:3.8 mixture of the cis- and trans-benzylmethylpyrrolidines II and III (R = H), whereas similar cyclization of I [R = Ph2P(O)] gave 81% of a 24:1 mixture of II and III [R = Ph2P(O)].

IT 281670-16-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(substituent effect in preparation of disubstituted pyrrolidines via diastereoselective radical cyclization of N-allyl β-amino selenides)

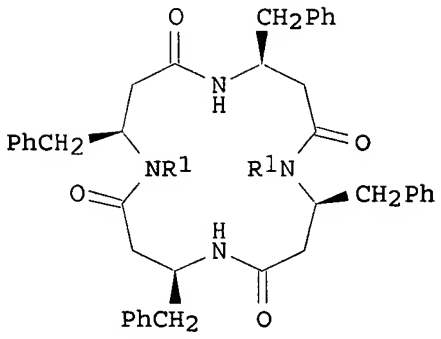
RN 281670-16-4 CAPLUS
CN Propanamide, N-[1-(phenylmethyl)-2-(phenylseleno)ethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)



RE.CNT 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:199899 CAPLUS
DN 130:312075
TI Design and synthesis of a novel cyclo-β-tetrapeptide
AU Sutton, Peter W.; Bradley, Adrian; Elsegood, Mark R. J.; Farras, Jaume; Jackson, Richard F. W.; Romea, Pedro; Urpi, Felix; Vilarrasa, Jaume
CS Departament de Quimica Organica, Universitat de Barcelona, Barcelona, 08028, Spain
SO Tetrahedron Letters (1999), 40(13), 2629-2632
CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.
DT Journal
LA English
GI



I

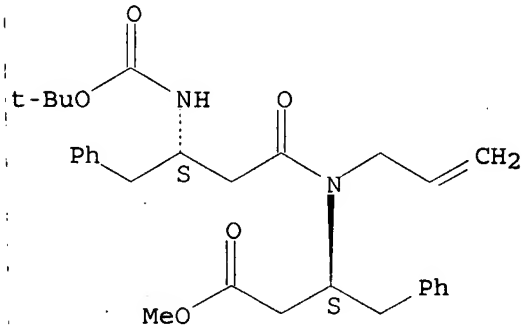
AB N-Substituted tetralactams (cyclo-β-tetrapeptides) have been identified as potential mol. scaffolds by computer-aided design; compound I (R1 = CH2CH:CH2), arising from L-β-homophenylalanine, has been prepared as a model system and its structure elucidated by single crystal X-ray anal. and NMR spectroscopy.

IT 223595-66-2P 223595-67-3P 223595-68-4P
223595-69-5P 223595-71-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design, synthesis, and conformation of a homophenylalanine derived cyclotetrapeptide)

RN 223595-66-2 CAPLUS

CN Benzenebutanoic acid, β-[[(3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

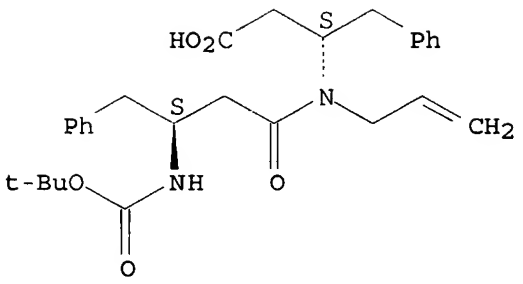
Absolute stereochemistry. Rotation (-).



RN 223595-67-3 CAPLUS

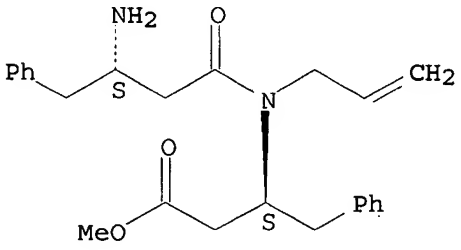
CN Benzenebutanoic acid, β-[[(3S)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 223595-68-4 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-, methyl ester, monohydrochloride, (βS)- (9CI) (CA INDEX NAME)

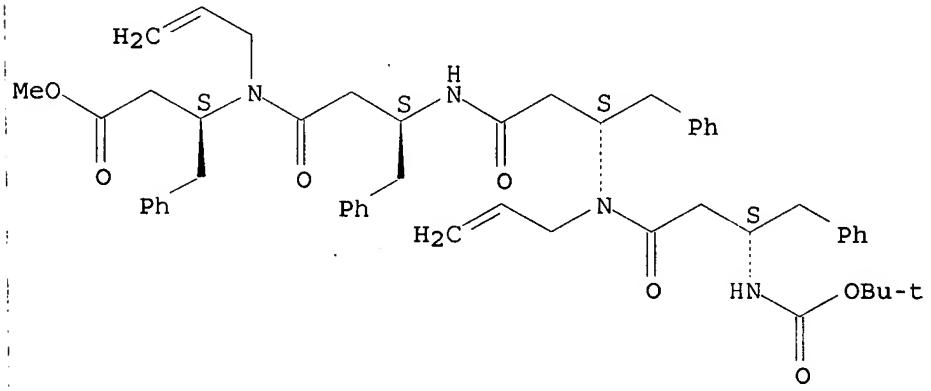
Absolute stereochemistry.



● HCl

RN 223595-69-5 CAPLUS
CN 2,6,10,14-Tetraazaheptadecanedioic acid, 5,9,13-trioxo-3,7,11,15-tetrakis(phenylmethyl)-6,14-di-2-propenyl-, 1-(1,1-dimethylethyl) 17-methyl ester, (3S,7S,11S,15S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

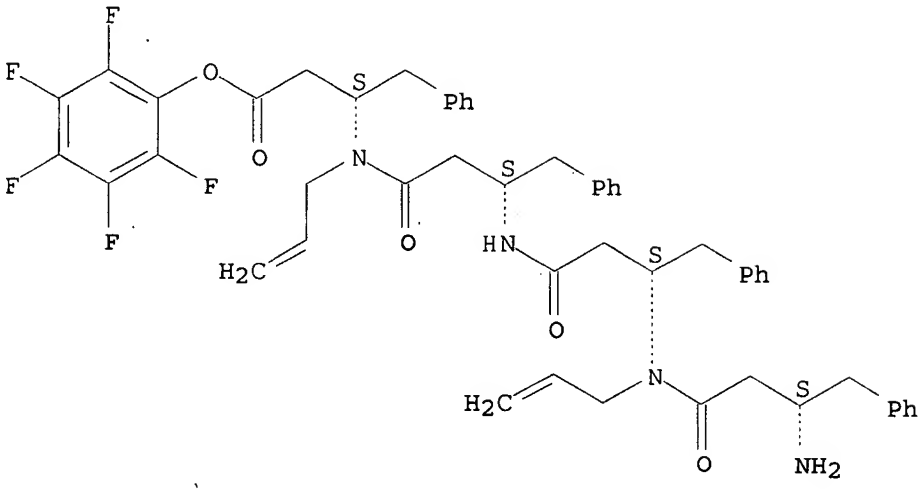


RN 223595-71-9 CAPLUS
CN Benzenebutanoic acid, β-[[(3S)-3-[[(3S)-3-[[(3S)-3-amino-1-oxo-4-phenylbutyl]-2-propenylamino]-1-oxo-4-phenylbutyl]amino]-1-oxo-4-phenylbutyl]-2-propenylamino]-, pentafluorophenyl ester, (βS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

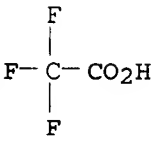
CRN 223595-70-8
CMF C52 H53 F5 N4 O5

Absolute stereochemistry.



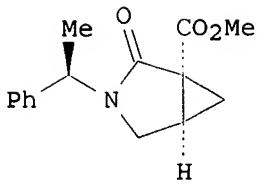
CM 2

CRN 76-05-1
CMF C2 H F3 O2

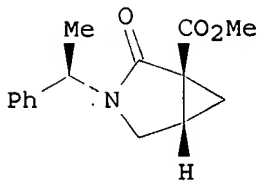


RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

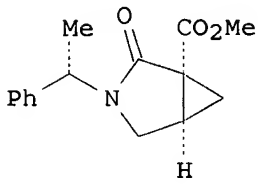
L31 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:763230 CAPLUS
DN 126:157356
TI Cyclization of (R)- and (S)-N-allyl-N-(1-phenylethyl)(methoxycarbonyl)acetamide mediated by Mn(III): preparation and structural assignment of 3-aza-2-oxobicyclo[3.1.0]hexanes
AU Galeazzi, Roberta; Geremia, Silvano; Mobbili, Giovanna; Orena, Mario
CS Dipartimento di Scienze dei Materali e della Terra, Universita di Ancona, Ancona, I-60131, Italy
SO Tetrahedron: Asymmetry (1996), 7(12), 3573-3584
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier
DT Journal
LA English
OS CASREACT 126:157356
GI



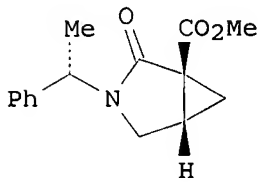
I



II



III



IV

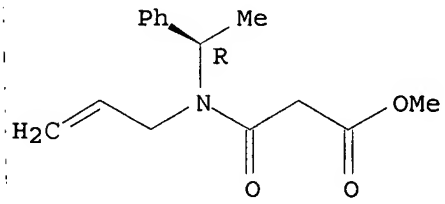
AB (R)- and (S)-N-allyl-N-(1-phenylethyl)(methoxycarbonyl)acetamide underwent oxidative cyclization mediated by Mn(III), to give easily separable diastereomeric mixts. of 3-aza-2-oxobicyclo[3.1.0]hexanes I, II, III, and IV, resp., whose structures were assigned on the basis of 1H NMR spectra and then confirmed by x-ray diffraction anal.

IT 186299-48-9P 186299-49-0P 186299-50-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azaoxobicyclohexanes by Mn-mediated cyclization of allyl(phenylethyl)(methoxycarbonyl)acetamides)

RN 186299-48-9 CAPLUS

CN Propanoic acid, 3-oxo-3-[(1-phenylethyl)-2-propenylamino]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

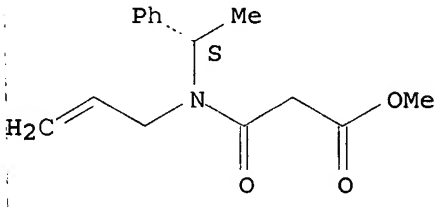
Absolute stereochemistry. Rotation (+).



RN 186299-49-0 CAPLUS

CN Propanoic acid, 3-oxo-3-[(1-phenylethyl)-2-propenylamino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

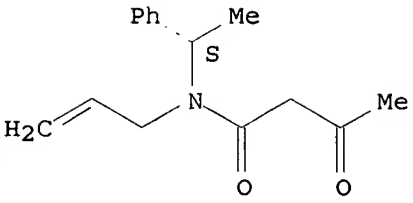
Absolute stereochemistry. Rotation (-).



RN 186299-50-3 CAPLUS

CN Butanamide, 3-oxo-N-[(1S)-1-phenylethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

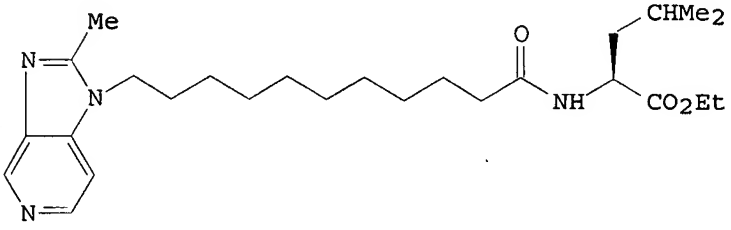


RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:77277 CAPLUS
DN 120:77277
TI Heterocyclic compound-substituted amino acid derivatives as PAF-receptor antagonists
IN Bowles, Stephen Arthur; Miller, Andrew; Whittaker, Mark
PA British Bio-Technology Ltd., UK
SO PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9314072	A1	19930722	WO 1993-GB9	19930106
	W: AU, CA, FI, JP, KR, NO, NZ, PT, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9332611	A	19930803	AU 1993-32611	19930106
	AU 661888	B2	19950810		
	EP 623116	A1	19941109	EP 1993-901058	19930106
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 07502742	T	19950323	JP 1993-512226	19930106
	US 5563151	A	19961008	US 1994-256140	19940901
PRAI	GB 1992-245	A	19920107		
	WO 1993-GB9	A	19930106		

OS MARPAT 120:77277
GI



I

AB The title compds. WZQN(R1)C(B)(R2)R3 [B = carbonyl derivative, carboxylate derivative, CH2OH, alkenyloxymethyl, alkynyloxymethyl, alkyloxymethyl, etc.; Q = CO, CS, SO2, direct bond; R1 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, (un)substituted Ph, etc.; R2 = H, halogen, (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, etc.; R3 = H, halogen; W = pyrid-3-yl, benzimidazol-1-yl, imidazo[4,5-c]pyridin-1-yl, imidazo[4,5-c]pyridinyl-3-yl, (un)substituted imidazo[4,5-c]pyridin-5-yl; Z = divalent alkanediyl, alkenediyl, alkynediyl, etc.], useful as platelet-activating factor receptor antagonists, are prepared Thus, N-11-(2-methylimidazo[4,5-c]pyridin-1-yl) undecanoyl-L-leucine Et ester I (colorless oil), was prepared from pentafluorophenyl 11-bromoundecanoate and demonstrated 50% inhibitory

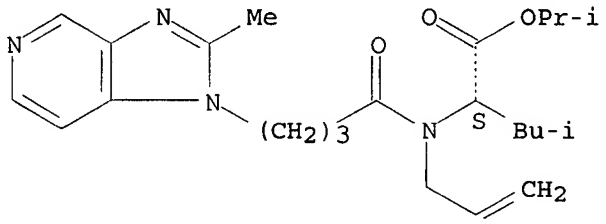
concentration for inhibition of tritiated platelet-activating factor binding to receptors isolated from human platelet plasma membranes of 1 nm.

IT 152550-69-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(platelet-activating factor receptor antagonist activity of)

RN 152550-69-1 CAPLUS

CN L-Leucine, N-[4-(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)-1-oxobutyl]-N-2-propenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1984:530424 CAPLUS

DN 101:130424

TI N-(α,α-Dialkylbenzyl)phenylacetamide compounds and herbicidal compositions containing them

IN Takematsu, Tetsuo; Kikkawa, Nobuyuki; Ogawa, Hideaki

PA Idemitsu Kosan Co., Ltd., Japan

SO U.S., 16 pp. Cont.-in-part of U.S. Ser. No. 118,746, abandoned.
CODEN: USXXAM

DT Patent

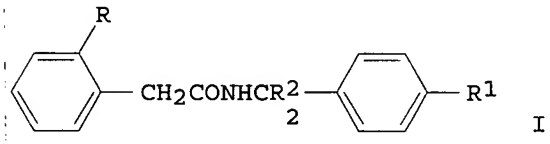
LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4455164	A	19840619	US 1982-366141	19820407
	JP 55104240	A	19800809	JP 1979-12211	19790207
	JP 57051827	B	19821104		
PRAI	JP 1979-12211	A	19790207		
	US 1980-118746	A2	19800205		

OS CASREACT 101:130424

GI



I

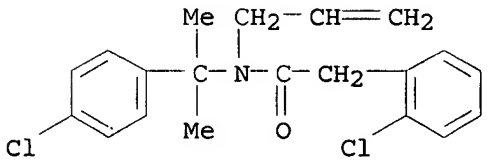
AB Amides I (R and R1 are Cl, Br; R2 = Me, Et), which were prepared, showed herbicidal activity. Thus, 2-ClC6H4CH2CO2H was treated with 4-ClC6H4CMe2NH2, Et3N, and 2-chloro-1-methylpyridinium iodide to give I (R = R1 = Cl, R2 = Me).

IT 80488-02-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicidal activity of)

RN 80488-02-4 CAPLUS

CN Benzeneacetamide, 2-chloro-N-[1-(4-chlorophenyl)-1-methylethyl]-N-2-

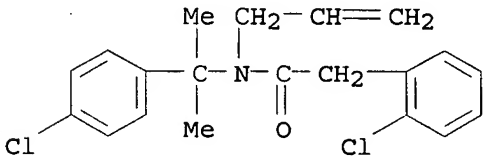
propenyl- (9CI) (CA INDEX NAME)



L31 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:52027 CAPLUS
DN 96:52027
TI N-(α,α-Dialkylbenzyl)phenylacetamide derivatives
PA Idemitsu Kosan Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 56110655	A	19810901	JP 1980-12413	19800206
	JP 58042864	B	19830922		
	JP 58043943	A	19830314	JP 1982-137181	19820809
PRAI	JP 1980-12413		19800206		

AB Forty-five title derivs. RC6H4CHR2CONR3CR4R5C6H5-n(R1)n I (R, R1 = H, halo, alkyl, alkoxy; R2 = H, alkoxy; R3 = H, alkyl, alkoxyalkyl, aryl; R4, R5 = alkyl; n = 1-3) were prepared Thus, refluxing 2-ClC6H4CH2CO2H 5, 4-ClC6H4CMe2NH2 5, Et3N 12, and 1-methyl-2-chloropyridinium iodide 6 mmol in CH2Cl2 gave 95.6% I (R = 2-Cl, R1 = 4-Cl, n = 1, R2 = R3 = H, R4 = R5 = Me) (II). II showed herbicidal activity at 200 g/acre.
IT 80488-02-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicidal activity of)
RN 80488-02-4 CAPLUS
CN Benzeneacetamide, 2-chloro-N-[1-(4-chlorophenyl)-1-methylethyl]-N-2-propenyl- (9CI) (CA INDEX NAME)



L31 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1975:427636 CAPLUS
DN 83:27636
TI Fungicidal aminonitriles
IN Kirino, Osamu; Oishi, Tadashi; Kameda, Nobuyuki; Kato, Toshiro; Fujinami, Akira; Itooka, Eiyoshi; Ozaki, Toshiaki
PA Sumitomo Chemical Co., Ltd., Japan
SO Ger. Offen., 58 pp.
CODEN: GWXXBX
DT Patent
LA German

FAN.CNT 1

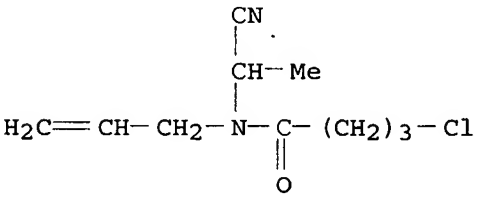
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2442239	A1	19750313	DE 1974-2442239	19740904
	JP 50049420	A	19750502	JP 1973-100547	19730905
	JP 51024569	B	19760724		
	JP 50101525	A	19750812	JP 1974-8358	19740117
	JP 53033657	B	19780916		
	JP 50101526	A	19750812	JP 1974-9450	19740121
	JP 50101530	A	19750812	JP 1974-10554	19740123
	JP 50105825	A	19750820	JP 1974-10555	19740123
	JP 52041330	B	19771018		
	ZA 7405500	A	19760428	ZA 1974-5500	19740827
	DK 7404678	A	19750505	DK 1974-4678	19740904
	NL 7411789	A	19750307	NL 1974-11789	19740905
	FR 2242374	A1	19750328	FR 1974-30201	19740905
	AU 7473017	A	19760311	AU 1974-73017	19740905
	US 3966789	A	19760629	US 1974-503425	19740905
PRAI	JP 1973-100547	A	19730905		
	JP 1974-8358	A	19740117		
	JP 1974-9450	A	19740121		
	JP 1974-10554	A	19740123		
	JP 1974-10555	A	19740123		

AB A series of 57 amino nitriles and cyanomethyl amides were prepared, resp., by Strecker synthesis and acylation of amino nitriles, and tested as fungicides for plants; extensive composition and test data were given. Compds. prepared and tested included, e.g., CH2:CHCH2NHCH2CN, n-C10H12NHCHMeCN, Cl(CH2)3CON(CH2CN)CH2CH:CH2, and p-ClC6H4CON(CH2CN)CH2CH:CH2.

IT 56095-98-8 56095-99-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(fungicidal activity of)

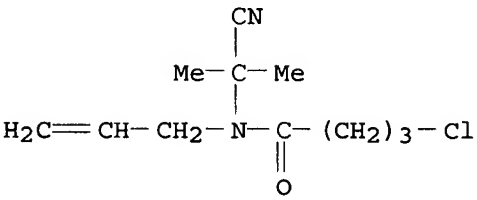
RN 56095-98-8 CAPLUS

CN Butanamide, 4-chloro-N-(1-cyanoethyl)-N-2-propenyl- (9CI) (CA INDEX NAME)



RN 56095-99-9 CAPLUS

CN Butanamide, 4-chloro-N-(1-cyano-1-methylethyl)-N-2-propenyl- (9CI) (CA INDEX NAME)



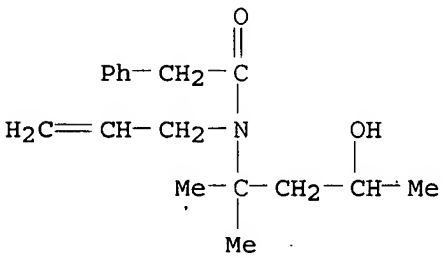
L31 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1974:82017 CAPLUS

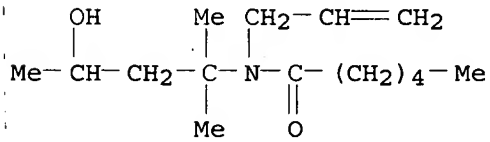
DN 80:82017

TI Claisen rearrangement of N-allylketene O, N-acetals

AU Ireland, Robert E.; Willard, Alvin K.
CS Gates and Crellin Lab. Chem., California Inst. Technol., Pasadena, CA, USA
SO Journal of Organic Chemistry (1974), 39(3), 421-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 80:82017
GI For diagram(s), see printed CA Issue.
AB Five N-(hydroxyalkyl)amides MeCH(OH)CH2CMe2N(CH2CH:CR2R3)COCHRR1 (R = Ph, Bu, hexyl; R1 = H, Me; R2 = H, Me; R3 = H, Me) are cyclized to dihydroxazines (I). The Claisen rearrangement of N-allylketene O,N-acetals (II) to I is discussed.
IT 43152-80-3 43152-81-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring closure of, rearrangement in, oxazine derivative from)
RN 43152-80-3 CAPLUS
CN Benzeneacetamide, N-(3-hydroxy-1,1-dimethylbutyl)-N-2-propenyl- (9CI) (CA INDEX NAME)



RN 43152-81-4 CAPLUS
CN Hexanamide, N-(3-hydroxy-1,1-dimethylbutyl)-N-2-propenyl- (9CI) (CA INDEX NAME)



L31 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1949:803 CAPLUS
DN 43:803
OREF 43:248g-i,249a-i,250a-i,251a-e
TI Acylglycinamides
IN Martin, Henry; Gysin, Hans
PA J. R. Geigy A.-G.
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2447587		19480824	US 1944-551636	19440828

GI For diagram(s), see printed CA Issue.
AB Dialkyl amides of α- or β-(monoalkylamino) carboxylic acids are obtained from an acid halide and the alkylamiao acid amide. Thus, ClCH2CONEt2 149.5 and EtNH2 100 g. in C6H6 300 mL. are autoclaved at 110-20°, cooled, filtered, and the filtrate washed with H2O and distilled to give N,N-diethyl-α-ethylaminoacetamide (I), b12 113-16°. Et2CHCOCl 13.4 added with cooling to I 31.6 g. in C6H6 100

mL. gives Et2CHCONEtCH2CONEt2, b0.3 134-6°. These and the following 329 compds. are soluble in both H2O and organic solvents, with few exceptions. They are useful as analeptics. The following examples are derivs. of α-amino acid amides. Compds. of the type REtNCH2CONMe2 (R given): Ac, b0.5 145-7°; iso-BuCO, b0.2 116-17°; Et2CHCO, b0.07 120-2°; Et2NCOCO, b0.18 159-61°; PhCH2CO, b0.3 195-7°; also MeAcNCH2CONMe2 b0.15 133°, m. 50-2°. REtNCH2CONEt2: Ac, b0.15 136-7°; iso-BuCO, b0.14 132-3°; Me3CCO, b0.15 124°, m. 61-2°; MeCCl:CHCO, b0.15 152-3°; Et2NCO, b0.33 139-40°; 2-AcOC6H4CO, b0.15 185-8°; 3,4-(MeO)2C6H3CO, b0.3 208-10°; MeC:N.O.C.Me:CCO, b0.6 170-2°, m. 74°; MeC:CH.CO.O.CMe:CCO, b0.5 212-15°, m. 105° RR'NCH2CONEt2 (R and R' given): Me, Ac, b0.05 128°; iso-Bu, Et2NCOCO, b0.16 174-5°; cyclopentyl, Me2NCOCO, b0.1 175-6°; cyclohexyl, Et2NCOCO, b0.1 200-3°, m. 80-1°. RMeNCHMeCONMe2: Ac, b0.04 103-5°; iso-BuCO(?), b0.3 135-8°; Me3CCO, b0.05 106-8°; Me3CCH2CO, b0.19 119°; MeCH:CHCO, b0.07 136-7°; MeCCl:CHCO, b0.15 132-4°; HC.tplbond.C(CH2)2CO, b0.1 135-6°. RMeNCHMeCONEt2: Ac, b0.2 101-3°; BuCO, b0.17 124-5°; iso-BuCO, b0.4 120-2°; Me3CCO, b0.25 108-10°; Me3CCH2CO, b0.2 118-20°; MeCH:CHCO, b0.015 117-18°; Me2NCO, b0.15 117°. REtNCHMeCONMe2: EtCO, b0.3 129-32°; iso-BuCO, b0.13 113-15°; Me3CCO, b0.1 114-16°; Et2CHCO, b0.25 123-5°; EtMeCHCH2CO, b0.15 121-2°; Me3CCH2CO, b0.03 110-12°; MeCH:CHCO, b0.11 123-5°; Me2C:CHCO, b0.1 128°; MeCCl:CHCO, b0.01 119-21°; Me(CH:CH)2CO, b0.15 166-8°; PrSCHMeCO, b0.2 142-3°; PrSCMe2CO, b0.4 180-2°; Me2CHC.tplbond.CCO, b0.09 132-4°; CH2.(CH2)4.CHCO, b0.35 142-4°; MeCH(CH2.CH2)2CHCO, b0.2 145-6°; O(CH2.CH2)2CHCO, b0.13 155-7°; 3,4-(MeO)2C6H3CH:CHCO, b0.4 205-8°. REtNCHMeCONMeEt: Me3CCO, b0.03 112-13°; MeCH:CHCO, b0.05 133-5°; Me2C:CHCO, b0.1 131-4°. REtNCHMeCONEt2: H, b11 105-7°; PrCO, b0.05 114-15°; BuCO, b0.1 122-3°; iso-BuCO, b0.15 129-30°; Me3CCO, b0.13 122°; Me3CCH2CO, b0.3 136-7°; MeCH:CHCO, b0.17 120-3°; Me2C:CHCO, b0.22 122-3°; Me2C:CMeCO, b0.09 118-20°; MeCCl:CHCO, b0.2 137-8°; Me(CH:CH)2CO, b0.7 156-8°; EtOCO, b0.5 117-18°; Et2NCO, b0.19 127-30°; Et2NCOCO, b0.08 146-7°; EtOCHMeCO, b0.2 134-5°; PrOCHMeCO, b0.08 130-2°; iso-PrOCHMeCO, b0.12 136-7°; EtOCHEtCO, b0.25 135°; 3,4-(MeO)2C6H3CO, b0.1 198-200°; O(CH2.CH2)2CHCO, b0.15 156-7°; HC:CH.CH:N.CH:CCO, b0.15 163-5°; MeC:N.O.CMe:CCO, b0.4 170-2°. REtNCHMeCON(CH2.CH2)2O: iso-BuCO, b0.26 155-7°; MeCH:CHCO, b0.02 156-8°. RPrNCHMeCONMe2: H, b15 110-12°; EtCO, b0.3 129-32°; PrCO, b0.15 126-9°; BuCO, b0.2 140-2°; iso-BuCO, b0.15 128-31°; Me3CCO, b0.24 122-5°; MeCH:CHCO, b0.1 129-31°; MeCCl:CHCO, b0.1 120-2°; Me2C:CHCO, b0.15 132°; Me2C:CMeCO, b0.3 138-41°. RPrNCHMeCONEt2: MeCH:CHCO, b0.25 136-8°; EtOCHMeCO, b0.2 125°. R(iso-Pr)NCHMeCONMe2: H, b15 90-2°; MeCH:CHCO, b0.1 121-2°, m. 82-5°; EtOCHMeCO, b0.2 131-3°. R(iso-Pr)NCHMeCONEt2: Ac, b0.04 113°; MeCH:CHCO, b0.02 138°, waxy; Me2C:CHCO, b0.25 142-4°. R(allyl)NCHMeCONMe2: BuCO, b0.1 120-1°; iso-BuCO, b0.27 122-4°; MeCH:CHCO, b0.05 127-8°; Me2C:CHCO, b0.1 122-4°. R(allyl)NCHMeCONEt2: H, b12 127-9°; iso-BuCO, b0.06 118-20°; MeCH:CHCO, b0.03 133°; Me2C:CHCO, b0.15 131-2°; Et2NCOCO, b0.08 169-70°. RBuNCHMeCONMe2: EtCO, b0.22 134°; iso-BuCO, b0.1 126-7°; MeCH:CHCO, b0.12 135-7°; Et2NCOCO, b0.35 180-2°. RBuNCHMeCONEt2: H, b12 125-30°; MeCH:CHCO, b0.13 141-3°; Me2C:CHCO, b0.07 140-2°; Me2NCOCO, b0.35 180-2°; Et2NCOCO, b0.08 164-6°. R(sec-Bu)NCHMeCONMe2: iso-BuCO, b0.25 129-31°; MeCH:CHCO, b0.5 144-6°; Me2C:CHCO, b0.45 149-51°.

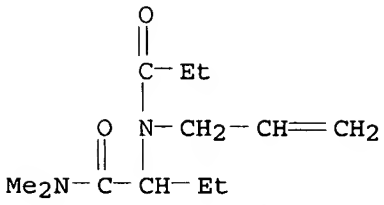
R(sec-Bu)NCHMeCONEt2: H, b11 112-15°; Me2C:CHCO, b0.3
135-7°; Et2NCOCO, b0.2 175-7°. EtCO(cyclopentyl)NCHMeCONMe2
b0.2 169-71°. R(cyclohexyl)NCHMeCONMe2 H, b12 162-4°; EtCO,
b0.1 165-7°. RMeNCHEtCONMe2: iso-BuCO, b0.01 117-19°;
MeCH:CHCO, b0.03 132-4°; PrSCMe2CO, b0.35 159-60°.
RMeNCHEtCONMeEt: iso-BuCO, b0.04 111-13°; MeCH:CHCO, b0.06
120-2°. RMeNCHEtCONEt2: H, b12 106-8°; iso-PrCO, b0.9
127-9°; iso-BuCO, b0.15 121-2°; Me3CCO, b0.25
110-12°; MeCH:CHCO, b0.09 128-30°; MeCCl:CHCO, b0.13
134°; Me2C:CHCO, b0.15 120-2°; Et2NCOCO, b0.16
158-9°; 3,4-(MeO)2C6H3CO, b0.08 203-5°. REtNCHEtCONMe2: H,
b12 100-1°; Ac, b0.6 126-7°; EtCO, b0.45 124-6°;
PrCO, b0.2 117°; iso-PrCO, b0.25 100-2°; BuCO, b0.1
128-9°; iso-BuCO, b0.1 121-4°; Me3CCO, b0.55 134-6°;
AmCO, b0.03 126-8°; Me2CHCHMeCO, b0.2 125°; Et2CHCO, b0.02
122-4°; Me3CCH2CO, b0.08 122-4°; Me(CH2)5CO, b0.2
132-4°; Et2CHCH2CO, b0.5 143-4°; MeCH:CHCO, b0.03
132-4°; MeCCl:CHCO, b0.09 131-3°; Me2C:CMeCO, b0.17
125-6°; Me2C:CHCO, b0.1 128°; Me(CH:CH)2CO, b0.35
145°; MeC.tplbond.CCO, b0.35 140-1°; EtOCHMeCO, b0.1
124°; PrOCHMeCO, b0.2 132-4°; iso-PrOCHMeCO, b0.03
132-3°, MeOCHEtCO, b0.1 125-6°; EtOCHEtCO, b0.3
143-5°; PrOCMe2CO, b0.1 134-6°; MeSCHMeCO, b0.1
144-5°; EtSCHMeCO, b0.17 150°; MeSCHEtCO, b0.4
160-2°; Et2NCOCO, b0.1 155°; O(CH2.CH2)2CHCO, b0.13
157°. REtNCHEtCONMeEt: PrCO, b0.1 126-7°; iso-BuCO, b0.1
114-15°; Me3CCO, b0.27 132-4°; MeCH:CHCO, b0.03
116-18°; Me2C:CHCO, b0.1 125-6°; EtOCHMeCO, b0.2
121-3°. REtNCHEtCONEt2: H, b15 111-14°; Ac, b0.08
107-8°; EtCO, b0.1 115°; PrCO, b0.1 124-6°; iso-PrCO,
b0.17 108°; BuCO, b0.1 124-6°; iso-BuCO, b0.15
120-2°; Me2CHCHMeCO, b0.12 125-6°; MeCH:CHCO, b0.3
136-8°; Me2C:CHCO, b0.17 130°; Me2C:CMeCO, b0.09
121-2°; MeCCl:CHCO, b0.15 134°; Me(CH:CH)2CO b0.15
146-8°; MeC.tplbond.CCO, b0.15 135-7°; EtC.tplbond.CCO, b0.1
138°; EtOCOCO, b0.3 140°; EtOCHMeCO, b0.05 122-3°;
Et2NCO, b0.05 115-17°; Me2NCOCO, b0.3 169-71°; Et2NCOCO,
b0.07 165-8°; 3,4-(MeO)2C6H3CO, b0.12 209-10°;
O(CH2.CH2)2CHCO, b0.35 173-5°; HC:N.CH:CH.CH:CCO, b0.15
162-4°; MeC:N.O.CMe:CCO, b0.35 170-1°, m. 55-6°;
MeC:CH.CO.N.CMe:CCO, b0.11 198-200°, m. 79-80°.
REtNCHEtCONPr2: iso-BuCO, b0.1 126-8°; Me2C:CHCO, b0.2 145°.
REtNCHEtCON(allyl)2: Ac, b0.05 124°; MeCH:CHCO, b0.1 130-2°;
Me2NCOCO, b0.12 170°. REtNCHEtCON(CH2.CH2)2O: PrCO, b0.11
140-2°; BuCO, b0.03 153°; iso-BuCO, b0.2 144-6°;
Me3CCH2CO, b0.02 149°; MeCH:CHCO, b0.04 155-8°; Me2C:CHCO,
b0.35 158-60°, m. 50-1°; Me(CH:CH)2CO, b0.12 165-7°,
waxy. REtNCHEtCON(CH2.CH2)2CH2: Me2C:CHCO, b0.06 154-5°; Et2NCOCO,
b0.65 195-6°, m. 82°. REtNCHEtCONR'R'' (given in order are
R, R', and R''). Et2NCOCO, Et, cyclohexyl, b0.05 188-90°;
Et2NCOCO, H, MeCH(CH2.CH2)2CH, b0.1 195-7°. Also
Et(Me2C:CHCO)NCHEtCON.(CH2)4.CHMe b0.15 165-7°.
RR'NCHR''CON(allyl)2 (given in order are R, R', and R''): Et, iso-BuCO,
Me, b0.2 130-2°; Me, Me2C:CHCO, Et, b0.2 128-30°.
RPrNCHEtCONMe2: H, b12 109-11°; Ac, b0.2 128-30°; EtCO, b0.2
119-20°; PrCO, b0.35 140-3°; iso-PrCO, b0.16 118°;
Me3CCO, b0.2 128°; MeCH:CHCO, b0.25 128-30°;
O(CH2.CH2)2CHCO, b0.3 175-6°. Pr(MeCH:CHCO)NCHEtCONEt2 b0.27
132-3°. R(iso-Pr)NCHEtCONMe2: Ac, b0.1 120-1°, m.
77-8°; EtCO, b0.3 126°; PrCO, b0.01 126-7°, m.
46-7°; MeCH:CHCO, b0.04 130°, m. 86-8°; EtOCHMeCO,
b0.1 124-5°; MeOCHEtCO, b0.2 123-5°. R(iso-Pr)NCHEtCONEt2:
H, b20 120-4°; iso-BuCO, b12 (or b0.12?) 123-6°; MeCH:CHCO,
b0.15 123-5°; Et2NCOCO, b0.25 150-2°; HC:CH.CH:N.CH:CHCO,

b0.25 170°, m. 77-8°. R(allyl)NCHEtCONMe2: Ac, b0.1 105°; EtCO, b0.1 114-16°; PrCO, b0.25 120-2°; iso-PrCO, b0.18 115-17°; BuCO, b0.17 127-9°; iso-BuCO, b0.25 125-7°; MeCH:CHCO, b0.2 132-4°; Me2C:CHCO, b0.15 122-4°; Me2C:CMeCO, b0.15 135°; EtOCHMeCO, b0.15 132-3°; iso-PrOCHMeCO, b0.08 130-2°. R(allyl)NCHEtCONEt2: H, b13 128-30°; MeCH:CHCO, b0.2 138-40°; Et2NCOCO, b0.22 171-3°. RBuNCHEtCONMe2: Ac, b0.15 121-2°; EtCO, b0.25 143-5°; iso-BuCO, b0.1 125-8°; MeCH:CHCO, b0.1 135°; Me2C:CHCO, b0.15 140-1°; Et2NCOCO, b0.45 180-2°; EtOCHMeCO, b0.12 130°; MeOCHEtCO, b0.1 128-30°. RBuNCHEtCONEt2: H, b13 135-8°; Me2NCOCO, b0.08 156°; Et2NCOCO, b0.08 164-6°. R(sec-Bu)NCHEtCONMe2: H, b13 112°; Ac, b0.01 117-18°; EtCO, b0.21 129-31°; MeCH:CHCO, b0.01 126-7°, m. 69-70°. RMeNCHPrCONEt2: Me2C:CHCO, b0.3 145-6°; Et2NCOCO, b0.4 178-80°. REtNCHPrCONMe2: PrCO, b0.015 119-20°; iso-BuCO, b0.2 130-2°; MeCH:CHCO, b0.08 130°, Me2C:CHCO, b0.25 139-41°; EtOCHMeCO, b0.1 135-7°; Et2NCOCO, b0.2 180-1°. REtNCHPrCONEt2: H, b12 121-4°; Ac, b0.15 125-6°. RPrNCHPrCONMe2: Ac, b0.15 120-2°; EtCO, b0.25 141-2°. Me(Et2NCOCO)NCH(iso-Pr)CONEt2 b0.1 152-3°, m. 68-9°. REtNCH(iso-Pr)CONMe2: Ac, b0.01 94°; MeCH:CHCO, b0.05 122-4°. REtNCH(iso-Pr)CONEt2: H, b12 108-10°; Et2NCOCO, b0.12 150-2°. RPrNCH(iso-Pr)CONMe2: Ac, b0.2 115-17°; EtCO, b0.1 113-15°; MeCH:CHCO, b0.1 130-2°. RMeNCHBuCONR'2 (given in order are R and R'): EtOCHMeCO, Me, b0.25 140-2°; Me2C:CHCO, Et, b0.2 144-5°. REtNCHBuCONMe2: H, b12 134-5°; Ac, b0.14 120-2°; EtCO, b0.2 135°; iso-BuCO, b0.1 126-8°; Me2C:CHCO, b0.1 140-1°; Me2C:CMeCO, b0.5 148-50°; Et2NCOCO, b0.45 190-2°. Et(iso-BuCO)NCHBuCONEt2 b0.3 135-8°. PrAcNCHBuCONMe2 b0.28 141-4°. REtNCHAmCONMe2: H, b12 128-30°; Ac, b0.06 136-7°. REtNCMe2CONEt2: H, b13 115-18°; iso-PrCO, b0.1 132-3°; Et2NCOCO, b0.2 167-70°; HC:CH.CH:N.CH:CCO, b0.3 175°; MeC:CH.CO.O.CMe:CCO, b0.15 210°. REtNCMeEtCONMe2: H, b13 118-20°; iso-PrCO, b0.5 128-30°. Other intermediates used in preparing certain of the preceding compds. are: EtNHCHEtCO2Et, b30 88-90°; Et(iso-BuCO)NCHEtCO2Et, b0.6 125-8°; NH2CHEtCONEt2, b12 109-11°; and PrCONHCHEtCONEt2, b0.2 180-2°. The following are derivs. of β-amino acid amides: REtN(CH2)2CONEt2: H, b13 124-7°; Me3CCO, b0.17 131-3°; MeCH:CHCO, b0.07 166°; Me2C:CHCO, b0.1 148-50°; Et2NCOCO, b0.07 166°; 3,4-(MeO)2C6H3CO, b0.08 207-10°; 2-AcOC6H4CO, b0.45 217-20°; HC:CH.CH:N.CH:CCO, b0.21 178-80°; MeC:N.O.CMe:CCO, b0.18 184-5°. Et(iso-BuCO)N(CH2)2CON(allyl)2 b0.08 155-6°. R(allyl)N(CH2)2CONEt2: H, b12 127-30°; Me2C:CHCO, b0.2 140-3°; Et2NCOCO, b0.12 168-9°. Allyl(iso-BuCO)N(CH2)2CONMe2 b0.2 125-8°. REtNCHMeCH2CONMe2: H, b12 105-6°; MeCH:CHCO, b0.1 135-6°. Also NH2CMe2CH2CONMe2 b12 107-10°; Me2C:CHCONHCMe2CH2CONMe2 b0.3 130-1°; and MeCH:CHCONHCMeEtCH2CONMe2 b0.3 135°. Cf. C.A. 41, 4804e, and preceding abstract

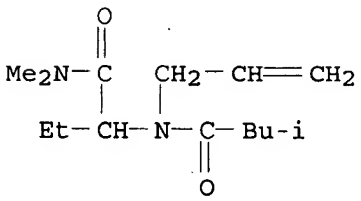
IT 854419-55-9P, Butyramide, 2-(N-allylpropionamido)-N,N-dimethyl- 854420-00-1P, Butyramide, N-allyl-N-(1-dimethylcarbamoylpropyl)-3-methyl- 854420-06-7P, Butyramide, N-allyl-N-(1-dimethylcarbamoylethyl)-3-methyl- 857976-32-0P, Valeramide, N-allyl-N-(1-dimethylcarbamoylethyl)- 857976-33-1P, Valeramide, N-allyl-N-(1-dimethylcarbamoylpropyl)- 861052-86-0P, Butyramide, 2-(N-allylbutyramido)-N,N-dimethyl- 875851-87-9P, Butyramide, N-allyl-N-(1-diethylcarbamoylethyl)-3-methyl-
RL: PREP (Preparation)
(preparation of)

RN 854419-55-9 CAPLUS

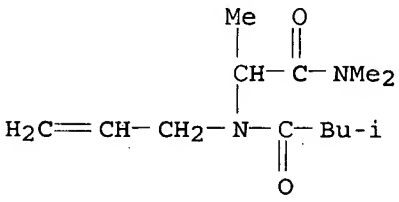
CN Butyramide, 2-(N-allylpropionamido)-N,N-dimethyl- (5CI) (CA INDEX NAME)



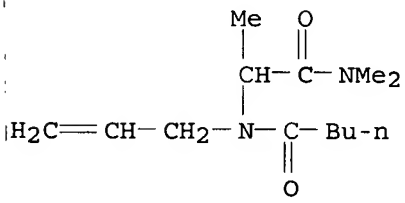
RN 854420-00-1 CAPLUS
CN Butyramide, N-allyl-N-(1-dimethylcarbamoylpropyl)-3-methyl- (5CI) (CA INDEX NAME)



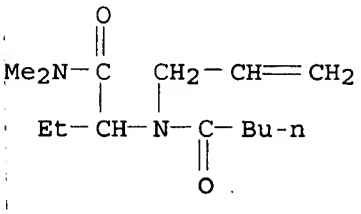
RN 854420-06-7 CAPLUS
CN Butyramide, N-allyl-N-(1-dimethylcarbamoylethyl)-3-methyl- (5CI) (CA INDEX NAME)



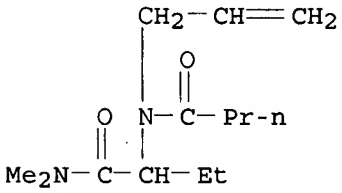
RN 857976-32-0 CAPLUS
CN Valeramide, N-allyl-N-(1-dimethylcarbamoylethyl)- (5CI) (CA INDEX NAME)



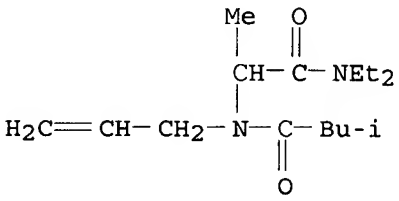
RN 857976-33-1 CAPLUS
CN Valeramide, N-allyl-N-(1-dimethylcarbamoylpropyl)- (5CI) (CA INDEX NAME)



RN 861052-86-0 CAPLUS
CN Butyramide, 2-(N-allylbutyramido)-N,N-dimethyl- (5CI) (CA INDEX NAME)



RN 875851-87-9 CAPLUS
CN Butyramide, N-allyl-N-(1-diethylcarbamoylethyl)-3-methyl- (5CI) (CA INDEX NAME)



L31 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1948:10381 CAPLUS
DN 42:10381
OREF 42:2272d-i,2273a-i,2274a-i,2275a-i,2276a-i,2277a-e
TI Acylated aliphatic amino carboxylic acid amides
PA J. R. Geigy A.-G.
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI GB 586135		19470307	GB 1943-21216	19431217

GI For diagram(s), see printed CA Issue.
AB Methods are described for the preparation of acylated aliphatic amino carboxylic acid amides and derivs. intended for therapeutic use as analeptics or solvent promoters. The compds. have the general formula R''R'NACONRR''' where R'' is alkyl or cycloalkyl, R' is the acyl radical of a carboxylic acid, A is alkylene, R is alkyl or cycloalkyl, and R''' is alkyl. ClCH2CONEt2 in C6H6 is heated with EtNH2 in an autoclave to 110-120°, cooled, filtered, mixed with H2O and KOH, and the C6H6 removed by distillation N,N-Diethyl-α-ethylaminoacetamide, rectified in vacuo, b12 113-16° and is miscible with H2O and organic solvents; when allowed to stand in C6H6 with Et2CHCOCl, filtered, freed from C6H6, poured into H2O, treated with alkalies, and rectified in vacuo it gives the compound Et2CHCONEtCH2CONEt2, b0.3 134-6°, miscible with H2O, Et2O, EtOH, and C6H6. In a similar manner N,N-diethyl-α-[(diethyloxamyl)isobutylamino]acetamide, b0.16 174-5°, miscible with H2O, EtOH, and Et2O, α-[cyclohexyl(diethyloxamyl)amino]-N,N-diethylacetamide, b0.1 200-3°, slightly miscible with water and miscible with organic solvents, and α-[cyclopentyl(dimethyloxamyl)amino]N,N-diethylamide, b0.1 175-6°, soluble in H2O and organic solvents, were prepared The following R'NEtCH2CONR2 are reported: R, R', B.p. °C. (m.m.), Form, Solubility W = H2O E = Et2O; Et, Me2CHCH2CO, 132-3, liquid, W easily soluble; , , (0.14), , E easily soluble; Et, Me3CCO, 124, solid, W easily

soluble; , , (0.15), m. 61-2°, E easily soluble; Me, Et2CHCO, 120-2, liquid, W miscible; , , (0.07), , E miscible; Me, Et2NCOCO, 159-61, liquid, W miscible; (0.18), , , E miscible; Me, Me2CHCO, 116-17, liquid, W miscible; , , (0.2), , E miscible; Et, 3,4-(MeO)2C6H3CO, 208-10, liquid, W easily soluble; , , (0.3), , E easily soluble; Et, o-AcOC6H4CO, 185-8, liquid, W easily soluble; , , (0.25), , E easily soluble, Et, MeC-CCO, 170-2, solid, W easily soluble; , N.O.CMe, (0.6), m. 74° E easily soluble; Et, CH:CMe.CCO, 212-15, solid, W easily soluble; , CO-O-CMe, (0.5), m. 105° E easily soluble; Et, Et2NCO, 139-40, liquid, W miscible; , , (0.33), , E miscible.; MeCH(NHMe)CONEt2 in C6H6 heated with Me2NCOCl 3 h. at 120° in an autoclave gives N,N-diethyl-α-[(dimethylcarbamyl)methylamino]propion amide, b0.15 117°, miscible with H2O and organic solvents. The following R'NMeCHMeCONR2 were prepared: R, R' B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et, BuCO, 124-5, liquid, W easily soluble; , , (0.17), , E easily soluble, Et*, Me2CHCH2CO, 120-2, liquid, W easily soluble; , , (0.4), , E easily soluble; Et, Me3CCO, 108-10, liquid, W easily soluble; , , (0.25), , E easily soluble; Et*, Me2CHCH2CO, 135-8, liquid, W moderately soluble; , , (0.3), , E easily soluble; *so given in original (?).; N,N-Diethyl-α-ethylaminopropionamide, b11 105-7°, is miscible with H2O and organic solvents, soluble in Et2O; treated dropwise with iso-BuCOCl, allowed to stand, filtered, separated from the Et2O, and distilled in vacuo, it gives N,N-diethyl-α-isovalerylaminopropionamide, b0.15 129-30°, miscible with H2O and organic solvents. The following R'NEtCHMeCONR2 are listed: R, R', B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et, PrCO, 114-15, liquid, W miscible; , , (0.05), , E miscible; Et, MeCH:CHCO, 120-3, liquid, W miscible; , , (0.17), , E miscible; Et, BuCO, 122-3, liquid, W easily soluble; , , (0.1), , E easily soluble; C3H5, Me2CHCH2CO, 130-2, liquid, W moderately soluble; , , (0.2), , E easily soluble; Me, Me2CHCH2CO, 113-15, liquid, W miscible; , , (0.13), , E miscible; Et, Me2C:CHCO, 122-3, liquid, W miscible; , , (0.22), , E miscible; Me, Me2C:CHCO, 128, liquid, W miscible; , , (0.10), , E easily soluble; Et, Me3CCO, 122, liquid, W soluble; , , (0.13), , E soluble; Me, Me3CCO, 114-16, liquid, W moderately soluble; , , (0.10), , E easily soluble; Et, Me2C:CMeCO, 118-20, liquid, W soluble; , , (0.09), , E soluble; Et, Et2NCOCO, 146-7, liquid, W miscible; , , (0.08), , E miscible; Et, 3,4-(MeO)2C6H3CO, 198-200, liquid, W soluble; , , (0.1), , E easily soluble; Et, , 163-5, liquid, W easily soluble; , , (0.15), , E easily soluble; Et, MeC-CCO, 170-2, liquid, W easily soluble; , N.O.CMe, (0.4), , E easily soluble; Et, Et2NCO, 127-30, liquid, W miscible; , , (0.19), , E miscible; Et, EtO2C, 117-18, liquid, W little soluble; , , (0.5), , E easily soluble, Et, MeCCl:CHCO, 137-8, liquid, W little soluble; , , (0.2), , E easily soluble; Me, Bz, 142-4, liquid, W soluble; , , (0.35), , E soluble; α-(Allylamino)-N,N-diethylpropionamide, b12 127-9°, in Et2O with iso-BuCOCl gives a product, b0.06 118-20°, moderately soluble in H2O, easily in Et2O; the analogous compound from β,β-dimethylacrylyl chloride b0.16 131-2°, is moderately soluble in H2O and easily soluble in Et2O. The acyl compound prepared from Et2NCOCO2H is soluble in H2O and Et2O and b0.08 169-70°. α-Butylamino-N,N-diethylpropionamide, b12 125-30°, miscible with H2O and organic solvents, gives with dimethylacrylyl chloride in ether a derivative, b0.07 140-2°, moderately soluble in H2O and organic solvents. Similar R'BuNCHMeCONR2 are given: R, R', B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et, MeCH:CHCO, 141-3, liquid, W moderately soluble; , , (0.13), E easily soluble; Me, Me2CHCH2CO, 126-7, liquid, W easily soluble; , , (0.1), , E easily soluble; Et, Me2NCOCO, 180-2, liquid, W soluble; , , (0.35), , E soluble; Et, Et2NCOCO, 164-6,

liquid, W moderately soluble; , , (0.08), , E easily soluble; α-sec-Butylamino-N,N-diethylpropionamide, b11 112-15°, miscible with H2O and organic solvents, with dimethylacrylyl chloride in ether gave a product b0.3 135-7°, soluble in H2O and Et2O. The diethyloxamyl derivative, b0.2 175-7°, is moderately soluble in H2O and easily soluble in Et2O. N,N-Diethyl-β-ethylaminopropionamide, b13 124-7°, miscible with H2O and organic solvents, with Me3CCOCl produced a derivative b0.17 131-3°, soluble in H2O and organic solvents. Other R'NEtCH2CH2CONR2 prepared: R, R', B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et, Et2NCOCO, 166, liquid, W easily soluble; , , (0.07), , E easily soluble; Et, MeCH:CHCO, 134-6, liquid, W easily soluble; , , (0.04), , E easily soluble; Et, Me2C:CHCO, 148-50, liquid, W easily soluble; , , (0.1), , E easily soluble; CH2CH:CH2, Me2CHCH2CO, 155-6, liquid, W moderately soluble; , , (0.08), , E easily soluble; Et, 3,4-(MeO)2C6H3CO, 207-10, liquid, W 10% soluble; , , (0.08), , E easily soluble; Et, , 178-80, liquid, W easily soluble; , , (0.21), , E easily soluble; Et, MeC-CCO, 184-5, liquid, W easily soluble; , N.O.CMe, (0.18), , E easily soluble; Et, o-AcOC6H4CO, 217-20, liquid, W 10% soluble; , , (0.45), , E easily soluble; β-(Allylamino)-N,N-diethylpropionamide, b12 127-30°, miscible with H2O and organic solvents, with dimethylacrylyl chloride in Et2O gives a derivative b0.2 140-3°, moderately soluble in H2O and easily soluble in organic solvents; diethyloxamyl derivative b0.12 168-9°. Isovaleric acid derivative b0.2 125-8°. N,N-Diethyl-α-(methylamino) butyramide, b12 106-8°, miscible with H2O and organic solvents, with dimethylacrylyl chloride in Et2O and C5H5N gives a product b0.15 120-2°, soluble in H2O and organic solvents. Derivs. of the general formula R'NMeCHEtCONR2 are listed: R, R', B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et, Me2CHCO, 127-9, liquid, W miscible; , , (0.9), , E miscible; Et, Me2CHCH2CO, , , 121-2, liquid, W moderately soluble; , , (0.15), , E easily soluble; C3H5, Me2C:CHCO, 128-30, liquid, W little soluble; , , (0.2), , E easily soluble; Et, Me3CCO, 110-12, liquid, W soluble; , , (0.25), , E easily soluble; Et; Et2NCOCO; 158-9; liquid; W easily soluble; , , (0.16); , E easily soluble; Et, 3,4-(MeO)2C6H3CO, 203-5, liquid, W little soluble; , , (0.08), , E easily soluble; α-Ethylamino-N,N-dimethylbutyramide, b12 100-1°, miscible with H2O and organic solvents, with iso-BuCOCl in ether gives a reaction product b0.1 121-4°, easily soluble in H2O and organic solvents. Other RNEtCHEtCONMe2 are given: R, B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Me2C:CHCO, 128, liquid, W easily soluble; , (0.1), , E easily soluble; Et2NCOCO, 155, liquid, W miscible; , (0.1), , E miscible; Me2C:CMeCO, 125-6, liquid, W easily soluble; , (0.17), , E easily soluble; MeCH:CHCH:CHCO, 145, liquid, W soluble; , (0.35), , E soluble; BuCO, 128-9, liquid, W soluble; , (0.1), , E soluble; Me(CH2)5CO, 132-4, liquid, W soluble; , (0.2), , E soluble; Me2CHCHMeCO, 125, liquid, W soluble; , (0.2), , E soluble; N,N-Diethyl-α-ethylaminobutyramide, b15 111-14°, miscible with H2O and organic solvents, stirred 2 h. with Et2NCOCOCl and the reaction product purified by distillation in vacuo, gives a colorless oil, b0.07 165-8°, soluble in H2O and organic solvents. Derivs. of the general formula R'NEt-CHEtCONRR0: NRR0, R', B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; NEt2, Ac, 107-8, liquid, W miscible; , (0.08), , E miscible; NEt2, EtCO, 115, liquid, W miscible; , , (0.1), , E miscible; NEt2, Me2CHCO, 108, liquid, W miscible; , , (0.17), , E miscible; NEt2, MeCH:CHCO, 136-8, liquid, W easily soluble; , , (0.3), , E easily soluble; NEt2, BuCO, 124-6, liquid, W moderately soluble; , , (0.1), E easily soluble; NEt2, Me2CHCH-MeCO, 125-6, liquid, W little soluble; , , (0.12), , E easily soluble; NEt2, Me2C:CHCO, 130, liquid, W 5% soluble; , , (0.17), E easily soluble; N(C3H52, Ac, 124, liquid, W moderately soluble; , , (0.05), , E easily soluble;

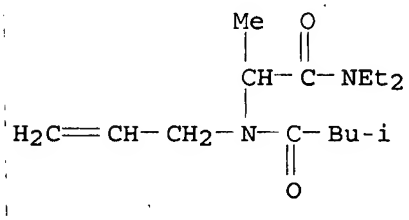
NEt2, Me2C:CMeCO, 121-2, liquid, W little soluble; , , (0.09), , E easily soluble;
NEt2, Me2NCOCO, 169-71, liquid, W miscible; , , (0.3), , E miscible;
N(C3H5)2, Me2NCOCO, 170, liquid, W soluble; , , (0.12), , E easily soluble; NEt2,
3,4-(MEO)2-C6H3CO, 209-10, liquid, W little soluble; , , (0.12), , E easily soluble; NEt2, , 162-4, liquid, W easily soluble; , (0.15), , E easily soluble;
NEt2, MeC-CCO, 170-1, liquid, W 5% soluble; , N.O.CMe, (0.33), , E easily soluble;
NEt2, CH:CMe.CCO, 198-200, liquid, W soluble; , CO. O . CMe, (0.11), , E easily soluble; NEt2, Et2NCO, 115-17, liquid, W easily soluble; CH2.CH2, (0.05), , E easily soluble; N CH2, Me2C:CHCO, 154-5, liquid, W difficultly soluble; CH2.CH2, ,
(0. 06), , E easily soluble; NPr2, Me2C:CHCO, 145, liquid, W difficultly soluble;
, , (0.2), , E easily soluble; NPr2, Me2CHCH2CO, 126-8, liquid, W little soluble;
, , (0.1), , E easily soluble; CH2.CH2, Et2NCOCO, 188-90, liquid, W little soluble; NEtCH CH2, , (0.05), , E easily soluble; CH2.CH2; NEt2, MeCCl:CHCO, 134, liquid, W little soluble; , , (0.15), , E easily soluble; NEt2, EtO2CCO, 140,
liquid, W difficultly soluble; , , (0.3), , E easily soluble; α-(Allylamino)-N,N-diethylbutyramide, b13 128-30°, miscible with water and organic solvents, with Et2NCOCOCl in Et2O gives a product, b0.22 171-3°, soluble in H2O and organic solvents; the crotonyl analog, moderately soluble in H2O
and easily soluble in organic solvents, b0.3 131-3°.
N,N-Diethyl-α-isopropylaminobutyramide, b20 120-4°, miscible with H2O and organic solvents, gives with iso-BuCOCl a product little soluble in
H2O, easily soluble in organic solvents, b12 123-6°. Derivs. of the general formula RN(iso-Pr)CHEtCONEt2: R, B.p. °C. (mm.), Solubility W = H2O E = Et2O; Et2NCOCO, 150-2, W approx. 10%; , (0.2), soluble in organic solvents; MeCH:CHCO, 123-5, W moderately soluble; , (0.15), E easily soluble, , 170, W soluble; N CO, (0.25), soluble in organic N solvents; α-Butylamino-N,N-diethylbutyramide, b13 135-8°, soluble in H2O and organic solvents, yields with Et2NCOCOCl a product moderately soluble in H2O and easily soluble in
organic solvents, b0.08 164-6°. Similar R'NBuCHEtCONR2 prepared: R, R', B.p. °C. (mm.), Solubility, Form, W = H2O E = Et2O; Me, Me2CHCH2CO, 125-8, liquid, W soluble; , , (0.1), , E easily soluble; Me, Me2C:CHCO, 140-1, liquid, W soluble; , , (0.15), , E easily soluble; Me, Et2NCOCO, 180-2, liquid, W
soluble; , , (0.45), , E soluble; Et, Me2NCOCO, 156, liquid, W soluble; , , (0.08), ,
E soluble; N,N-Diethyl-α-ethylaminoisobutyramide, b13 115-18°, miscible with H2O and organic solvents, gives with iso-PrCOCl a product b0.1 132-3°, easily soluble in H2O and organic solvents. Other compds. of the general formula RNECMe2CONEt2 were made: R, B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et2NCOCO, 167-70, liquid, W miscible, , (0.2), , E miscible; CO, 175, liquid, W miscible; N, (0.3), , E miscible; CH:CMe.CCO, 210, liquid, W easily soluble; CO . O . CMe; (0.15), , E easily soluble; N, N-Diethyl-α-ethylaminoisovaleramide, b12 108-10°, with Et2NCOCOCl yielded a compound b0.12 150-2°, solubility in water about 5%, easily soluble in Et2O. N,N-Diethyl-α-methylaminoisovaleramide yields a solid, m. 68-9°, b0.1 152-3°, about 5% soluble in H2O, easily soluble in organic solvents. N,N-Diethyl-α-ethylaminovaleramide, b12 121-4°, soluble in H2O and organic solvents, gives with AcCl a compound, b0.15 125-6°, moderately soluble in H2O and easily soluble in organic solvents. Compds. of the general formula R''R'NCH-PrCONR2 are given: R, R', R'', B.p. °C. (mm.), Form, Solubility W = H2O E = Et2O; Et, Et2NCOCO, Me, 178-80, liquid, W soluble; , , , (0.4), , E soluble; Me, Me2C:CHCo,
Et, 139-41, liquid, W soluble; , , , (0.25), , E soluble; Et, Et2NCOCO, Et, 180-1,

liquid, W moderately soluble; , , , (0.2), , E soluble; Me, Me2CHCH2CO, Et, 130-2,
liquid, W soluble; , , , (0.2), , E soluble; Et, Me2C:CHCO, Me, 145-6, liquid, W
moderately soluble; , , , (0.3), , E easily soluble; α-Ethylamino-N,N-dimethylcaproamide, b12 134-5°, soluble in water and organic solvents, forms with iso-BuCOCl a product b0.1 126-8°, soluble in H2O and organic solvents. The general formula R''R'NCHBuCONR2 represents the following compds.: R, R', R'', B.p. °C.(mm.), Form, Solubility W = H2O E = Et2O; Et, Me2C:CHCO, Me, 144-5, liquid, W little soluble; (0.2), E easily soluble; Et, Me2CHCH2CO, Et, 135-8, liquid, W little soluble; (0.3), E easily soluble; Me, Me2C:CHCO, Et, 140-1, liquid, W soluble; (0.1), E soluble; Me, Me2C:CMeCO, Et, 148-50, liquid, W soluble; (0.5), E soluble; Me, Et2NCOCO, Et, 190-2, liquid, W soluble; (0.45), E soluble; EtCHBrCO2Et heated with an excess of EtNH2 in C6H6 in an autoclave 6 h. at 80° gives Et α-ethylamino-butyrate, b30 88-9°, which, allowed to react in Et2O with iso-BuCOCl at room temperature for several hrs., yields Et α-(ethylisovalerylamino)butyrate, b0.6 125-8°. The ester, refluxed with NaOH in EtOH 2 h., diluted with H2O, freed from EtOH, extracted with Et2O, made acid to Congo red, the Et2O removed by distillation, the mixture treated with PCl5 at room temperature, the
POCl3 removed by distillation, and the residue treated in Et2O with NHEt2 yields
a product, b0.15 120-2°, moderately soluble in H2O and easily soluble in organic solvents. α-Amino-N,N-diethylbutyramide, b12 109-11°, miscible with H2O and organic solvents, stirred several hrs. with PrCOCl, filtered, and distilled in vacuo, yields α-butyrylamino-N,N-diethylbutyramide, b0.2 180-2°, which, heated to boiling in xylene with sodamide, cooled, treated with EtI, heated in an autoclave until reaction is completed, filtered, and rectified in vacuo, gives a product b0.1 124-6°, moderately soluble in H2O, easily soluble in organic solvents.

IT 875851-87-9P, Butyramide, N-allyl-N-(1-diethylcarbamoylethyl)-3-methyl-
RL: PREP (Preparation)
(preparation of)

RN 875851-87-9 CAPLUS

CN Butyramide, N-allyl-N-(1-diethylcarbamoylethyl)-3-methyl- (5CI) (CA INDEX NAME)

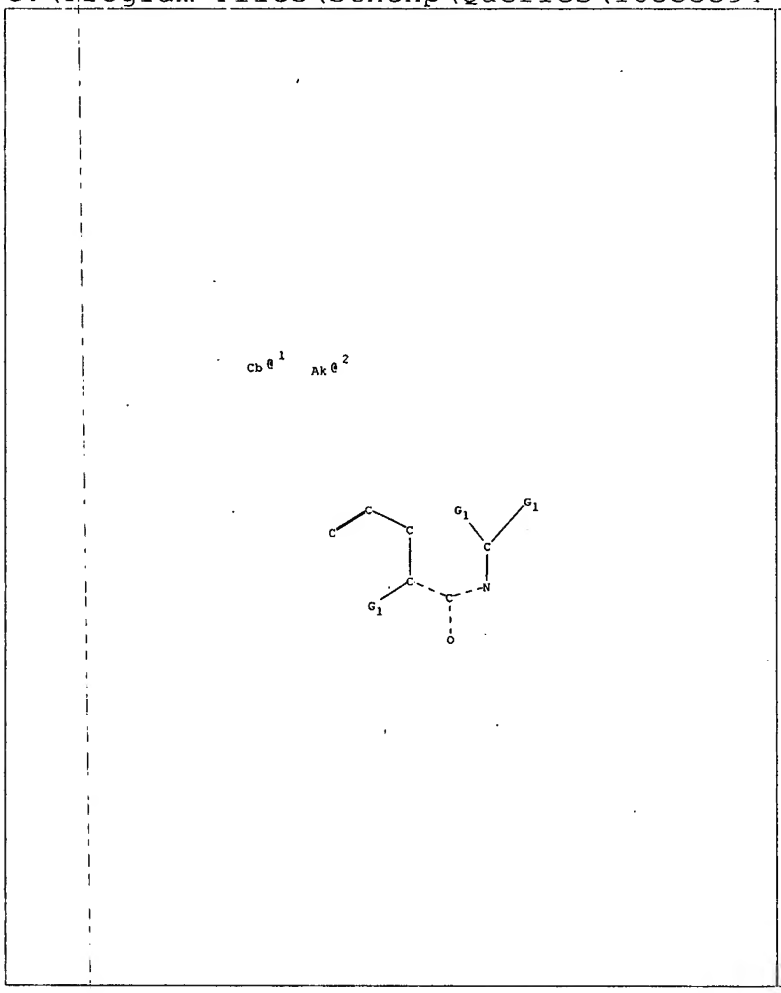


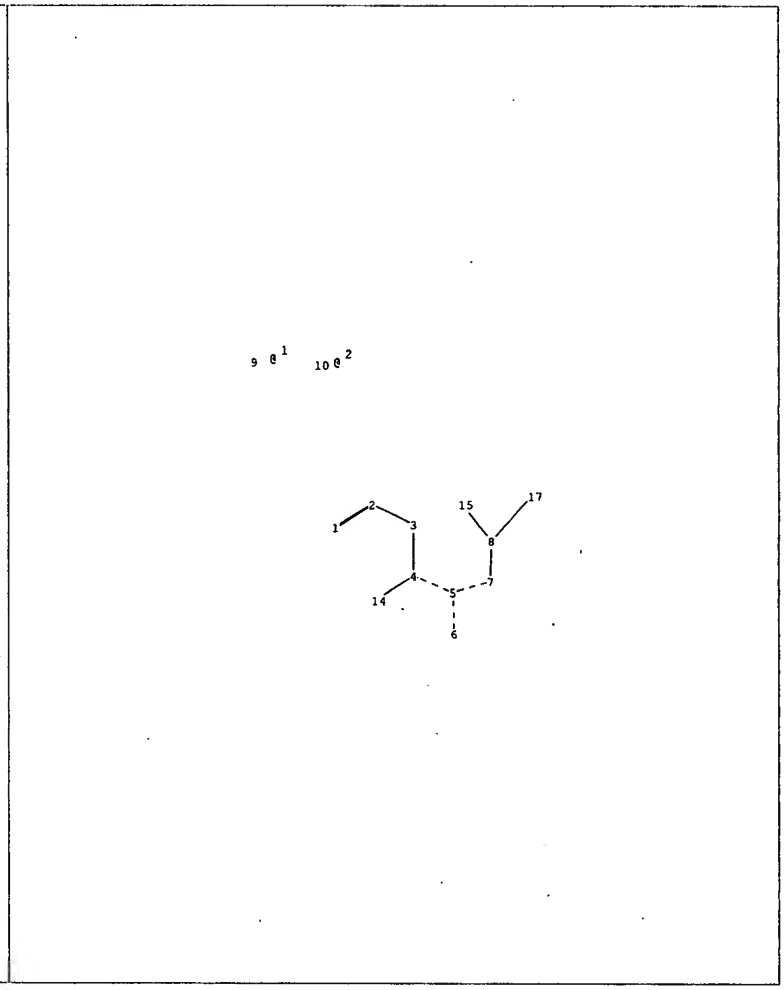
=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	90.06	752.80
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-13.26	-32.39

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:55:40 ON 21 MAY 2007

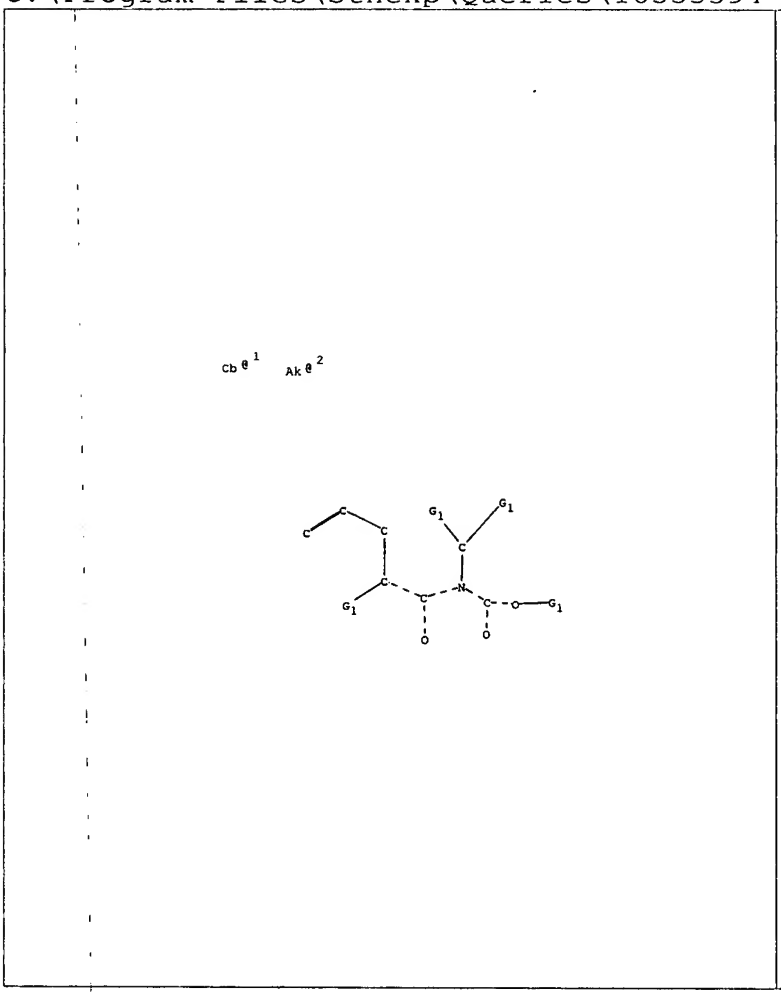
C:\Program Files\Stnexp\Queries\10553394-intermd.str

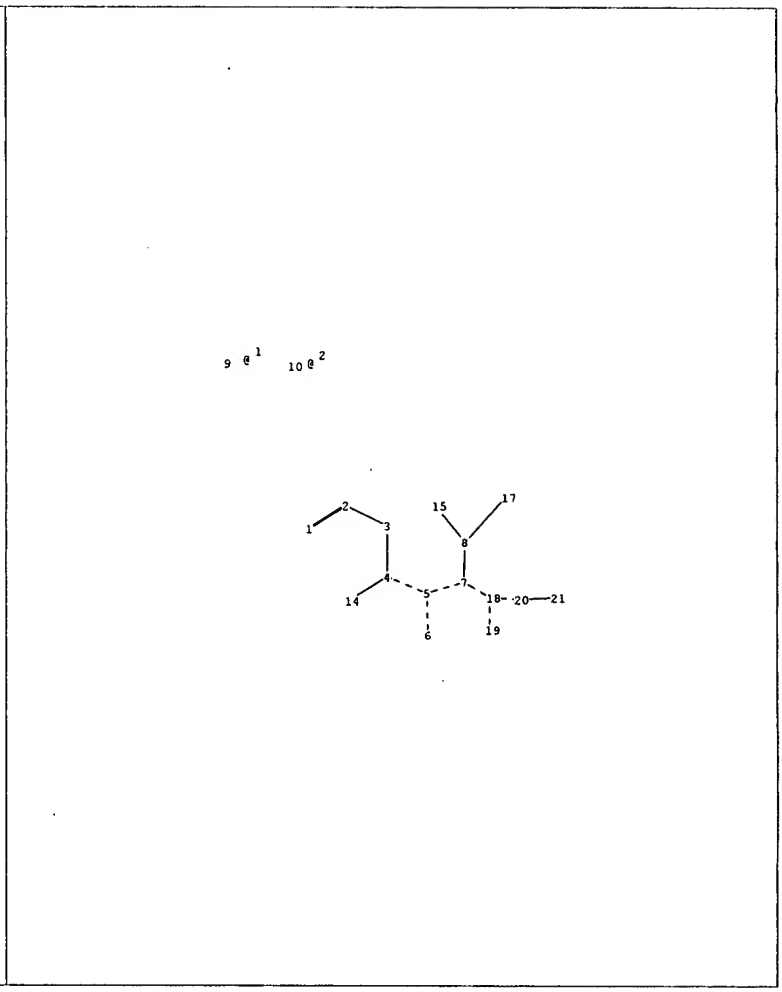





```
chain nodes :
    1   2   3   4   5   6   7   8   9  10  14  15  17
chain bonds :
    1-2  2-3  3-4  4-5  4-14  5-6  5-7  7-8  8-15  8-17
exact/norm bonds :
    1-2  2-3  3-4  4-5  4-14  5-6  5-7  7-8  8-15  8-17

G1:[*1],[*2]

Match level :
    1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS
    9:Atom  10:CLASS  14:CLASS  15:CLASS  17:CLASS
Generic attributes :
    9:
    Saturation              : Unsaturated
    10:
    Saturation              : Saturated
```

C:\Program Files\Stnexp\Queries\10553394-interm3.str



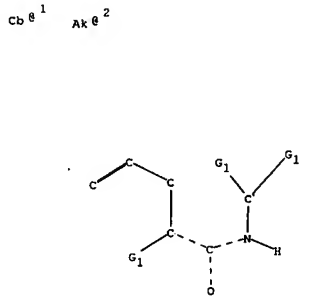


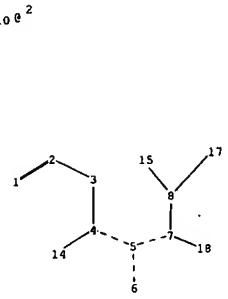
chain nodes :
1 2 3 4 5 6 7 8 9 10 14 15 17 18 19 20 21
chain bonds :
1-2 2-3 3-4 4-5 4-14 5-6 5-7 7-8 7-18 8-15 8-17 18-19 18-20
20-21
exact/norm bonds :
1-2 2-3 3-4 4-5 4-14 5-6 5-7 7-8 7-18 8-15 8-17 18-19 18-20
20-21

G1:[*1],[*2]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
9:Atom 10:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS
Generic attributes :
9:
Saturation : Unsaturated
10:
Saturation : Saturated

C:\Program Files\Stnexp\Queries\10553394-interm6.str



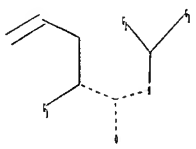


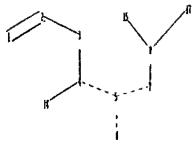
chain nodes :
1 2 3 4 5 6 7 8 9 10 14 15 17 18
chain bonds :
1-2 2-3 3-4 4-5 4-14 5-6 5-7 7-8 7-18 8-15 8-17
exact/norm bonds :
1-2 2-3 3-4 4-5 4-14 5-6 5-7 7-8 7-18 8-15 8-17

G1:[*1],[*2]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
9:Atom 10:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS
Generic attributes :
9:
Saturation : Unsaturated
10:
Saturation : Saturated

```
=>
Uploading C:\Program Files\Stnexp\Queries\10553394-intermd.str
```





```
chain nodes :
1  2  3  4  5  6  7  8  9  10  14  15  17
chain bonds :
1-2  2-3  3-4  4-5  4-14  5-6  5-7  7-8  8-15  8-17
exact/norm bonds :
1-2  2-3  3-4  4-5  4-14  5-6  5-7  7-8  8-15  8-17

G1:[*1],[*2]

Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:Atom
10:CLASS
14:CLASS  15:CLASS  17:CLASS
Generic attributes :
9:
Saturation              : Unsaturated
10:
Saturation              : Saturated


L9      STRUCTURE UPLOADED

=> s l9
SAMPLE SEARCH INITIATED 17:10:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    73318 TO ITERATE
```